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Path integral treatment of systems with general memory: Application to the Bose polaron problem

Padintegraalbeschrijving van systemen met algemeen geheugen: een toepassing op het Bose-polaron probleem.

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Samenvatting

Dit proefschrift situeert zich in het domein van de fysica van de gecondenseerde materie, die breed kan worden gedefinieerd als de studie van hoe de macroscopische eigenschappen van materie, zoals vaste stoffen, vloeistoffen of zelfs meer exotische fasen, onstaan als gevolg van het gedrag van de microscopische bestanddelen ervan. De grootste moeilijkheid bij de meeste vraagstukken in dit domein komt neer op het uitzoeken hoe interacties een invloed uitoefenen op de verschillende delen van het systeem die op zichzelf goed begrepen zijn. Inderdaad, terwijl de meeste fysicastudenten de exacte kwantummechanische oplossing voor het gedrag van een waterstofatoom op een stukje papier kunnen neerschrijven, wordt voor een wolkje van honderden atomen dezelfde taak hopeloos zelfs met behulp van krachtige supercomputers. Het doel van de fysicus is daarom, misschien in tegenstelling tot wat vaak wordt gedacht, niet zozeer om altijd exacte oplossingen te vinden maar eerder om te begrijpen welke processen essentieel zijn en hierrond juiste benaderingen te kunnen maken. Speelt het gedrag van de atoomkern nu echt een grote rol bij het begrijpen van de meeste eigenschappen van ons wolkje atomen?

Een interessante klasse van problemen die in deze thesis aan bod zullen komen situeren zich in het deeldomein van polaronische fysica, waarbij een klein systeem dat in wisselwerking staat met een groot extern systeem bestudeerd kan worden als een onzuiverheid die wordt ingebracht in een medium of omgeving. De onzuiverheid verstoort het medium en vormt een quasideeltje dat bestaat uit de onzuiverheid samen met een wolk van excitaties van het medium, ook wel een *polaron* genoemd. Het concept van een polaron is voor het eerst geïntroduceerd, en bleek ook enorm succesvol te zijn, om de eigenschappen te beschrijven van een elektron dat door een ionenrooster van een kristal beweegt. Hoewel polaronen nu al bijna een eeuw in verschillende fysische systemen worden bestudeerd, werd het domein in een geheel nieuwe richting geduwd door de recente experimenten waarbij polaronen zijn gemaakt door onzuiverheidsatomen in te brengen in Bose-Einstein-condensaten.

De theoretische beschrijving van het Bose-polaron is om een aantal redenen bijzonder uitdagend. De grote experimentele vrijheid in ultrakoude atomaire gassen maakt het mogelijk om meer systeemparameters in te stellen en omstandigheden te creëren waarin nieuwe soorten interactieprocessen tussen de onzuiverheid en het condensaat belangrijk worden, die voorheen niet werden aangetroffen in andere polaronische systemen. Afgezien van deze uitbreiding blijkt het Bose-polaron ook meer kwantummechanisch gedrag te vertonen dan zijn tegenhanger in vaste stoffen, wat nieuwe theoretische moeilijkheden veroorzaakt. Er is bijvoorbeeld aangetoond dat Feynmans variationele padintegraalmethode, die tot nu toe de theoretische voorkeursmethode was voor het bestuderen van polaronen in de vastestoffysica, niet in staat is om het Bose-polaron te beschrijven.

Gemotiveerd door dit probleem, is het doel van deze thesis om drie uitbreidingen van de padintegraalmethode te bestuderen die de bestaande tekortkomingen aanpakken en verbeteren in verschillende richtingen. In overeenstemming hiermee worden de meest opvallende resultaten van het proefschrift ook gepresenteerd met de nadruk op padintegratiemethoden, terwijl het Bose-polaronprobleem eerder de leidraad zal vormen. Vooral in de tweede helft van de thesis zal duidelijk blijken dat sommige van de methoden bredere toepassingen zouden kunnen hebben dan alleen in de polaronfysica, in het bijzonder in de context van open kwantumsystemen of variationele methoden voor veeldeeltjes systemen.

Hoofdstuk 1 van dit proefschrift bestaat uit een korte inleiding tot de polaronfysica. Na een overzicht te geven van de rijke geschiedenis van dit domein, zal het Bose-polaronprobleem van een onzuiverheid in een condensaat worden besproken. In het bijzonder zal de nadruk liggen op de verschillende experimenten en theoretische modellen die zijn gebruikt om dit systeem te bestuderen.

In hoofdstuk 2 beginnen we met de bespreking van het falen van Feynmans variationele padintegraalmethode voor het Bose-polaronprobleem – iets dat recent veel aandacht heeft gekregen in de literatuur. We beschouwen een aantal mogelijke uitbreidingen en tonen aan dat de padintegraalmethode voor dit probleem in twee stappen enorm verbeterd kan worden. Er wordt aangetoond dat de nieuwe aanpak uitstekend overeenkomt met rigoureuze diagrammatische Monte Carloberekeningen, wat dus bevestigt dat de padintegraalmethode kan worden gebruikt om dit uitdagendere polaronische systeem te bestuderen.

Om polaron vorming in Bose gassen te beschrijven, moet er ook rekening worden gehouden met verstrooiingsprocessen van hogere orde tussen de onzuiverheden en excitaties in het gas, wat niet beschreven wordt door het voorheen veel bestudeerde Fröhlich-model. In hoofdstuk 3 wordt een methode gepresenteerd om een hersommatie van deze hogere-orde processen op het niveau van de effective polaronactie uit te voeren, en wordt dit vervolgens toegepast op een enkelvoudig Bose-polaron.

In de experimenten worden de onzuiverheden in eindige aantallen gecreëerd en zijn ze bovendien bosonisch of fermionisch. Het is daarom noodzakelijk om voorzichtig te zijn met deeltjesstatistiek en na te gaan wanneer deze in rekening gebracht moet worden. In het laatste deel van deze thesis richten we ons op het ontwikkelen van een kader waarin het mogelijk zou zijn om dit soort problemen aan te pakken, terwijl de vrijheid over het type omgeving zeer algemeen moet kunnen blijven in lijn met de bevindingen van Hoofdstuk 2. Hiervoor wordt in Hoofdstuk 4 een formalisme gepresenteerd om bosonen met algemene geheugenkernels in het canonische ensemble te beschrijven. Deze benadering wordt vervolgens uitgebreid naar één-en tweepuntscorrelatiefuncties in Hoofdstuk 5. De belangrijkste focus van de discussie is gericht op variationele modellen van kwantumsystemen met meerdere deeltjes in een omgeving, waarvan Bose-polaronen een voorbeeld kunnen zijn.

Ten slotte combineren we de verschillende methoden uit deze thesis in Hoofdstuk 6 om een aantal grondtoestandseigenschappen van een eindig aantal Bose-polaronen bij nultemperatuur te bestuderen. We bespreken het belang van de voorgenoemde hogere-orde verstrooiingsprocessen en vinden dat voor meerdere onzuiverheden zelfs bij zwakke interacties deze processen een cruciaal stabiliserend effect vertonen.

Abstract

This thesis is situated in the field of condensed matter physics which can be broadly defined as the study of how the macroscopic properties of matter such as solids, liquids or even more exotic phases arise following from the behavior of its microscopic constituents. The main difficulty in almost any condensed matter problem comes down to figuring out how interactions affect different parts of the system that are by themselves well understood. Indeed, while any undergraduate physics student can write down the exact quantum mechanical solutions for the behavior of a hydrogen atom on a piece of paper, for hundreds such atoms this same task becomes hopeless even with the aid of powerful supercomputers. The goal of the physicist is therefore, perhaps contrary to popular belief, to make approximations to the system that capture the processes that are essential for the phenomenon of interest and neglect those that are not. Does the behavior of the atomic nucleus really play a role in understanding the average properties of our collection of atoms?

One interesting class of problems that will be studied in this thesis is found in the subdomain of polaronic systems, where a small system of interest that is interacting with a large external system is studied through the lens of an impurity being immersed in a medium. The impurity disturbs the medium and together with a surrounding cloud of excitations of the medium forms a quasiparticle called a *polaron*. The concept of a polaron has first been introduced to understand the properties of an electron moving through an ionic lattice of a solid crystal for which it proved to be extremely successful. Although polarons have now been studied for nearly a century in various physical systems, recent experiments where polarons have been created by immersing impurity atoms in Bose-Einstein condensates have pushed the domain in a completely new direction.

The theoretical description of the Bose polaron is particularly challenging for a couple of reasons. The great experimental freedom in ultracold atomic gases allows one to create conditions where novel types of interaction processes between the impurity and condensate, that have previously not been encountered in other polaronic systems, now become important. Aside from this extension, the Bose polaron also seems to exhibit more quantum mechanical properties than its solid state counterpart which creates new theoretical difficulties. In particular, Feynman's variational path integral treatment, that has thus far been the theoretical method of choice in the description of polarons in solid state physics, has been shown to fail to describe the Bose polaron.

Motivated by this problem, the aim of the thesis is to study three extensions of the path integral approach that address the current shortcomings and improve upon them in various directions. In accordance, the most notable results of the thesis are also presented with an emphasis on path integration methods, whereas the Bose polaron problem will act as a guide towards points of improvement. Especially towards the latter half of the thesis it will be shown that some of the methods could have wider applications than just in polaron physics, in particular in the context of open quantum systems or many body variational models.

Chapter 1 of this thesis consists of a brief introduction to polaron physics for the unfamiliar reader. After providing an overview of the rich history of this field, the Bose polaron problem of an impurity in a condensate will be discussed. In particular, the focus will lie on the various experiments and theoretical models that have been used to study this system.

In Chapter 2 we start by discussing the failure of Feynman's variational path integral approach to the Bose polaron problem which has received significant attention in the literature in the past decade. We proceed by considering a number of extensions and show that the path integral approach to this problem can be tremendously improved in two steps that have been shown to produce only minor corrections in previous solid state polaron studies. We show that the new approach is in excellent agreement with rigorous diagrammatic Monte Carlo calculations and establish that the path integral approach is capable of capturing the physics of this more challenging polaronic system.

To describe polaron formation in Bose gases, higher-order scattering events between the impurities and excitations in the gas have to be taken into account, which requires one to go beyond the well-studied Fröhlich model. In Chapter 3, a method is presented to perform a resummation of these higher-order scattering events at the level of the effective polaron action, and is subsequently applied to a single Bose polaron.

In the experiments the impurities are created at finite number and are either bosonic or fermionic. It is therefore necessary to be cautious with particle statistics and confirm case by case when such effects can be neglected. The final aim of the thesis is to develop a framework that would allow us to tackle these types of problems while keeping the freedom on the type of environment sufficiently general, in accordance with the findings in Chapter 2. For this purpose, in Chapter 4 a formalism to describe bosons with general memory kernels in the canonical ensemble is presented. This approach is then extended towards one and two-point correlation functions in Chapter 5. The main focus of the discussion is aimed towards a generalization of previous path integral techniques and an application to open quantum systems of identical particles, of which Bose polarons could be one example.

Finally, in Chapter 6 we apply the many-impurity generalized approach to study a number of properties of a finite number of Bose polarons at zero temperature. We discuss the importance of the aforementioned higher-order scattering events for multiple impurities and find that even at weak coupling they provide a crucial stabilizing effect.

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CHAPTER

Polarons

Polarons have a long-standing history of study across multiple physical systems requiring various theoretical techniques for their description. This chapter presents a general overview of the topic and introduces useful concepts that reoccur throughout the thesis. After covering the early history of polarons and their first theoretical models, the emphasis is placed on the Bose polaron and its differences with the solid state polaron.

1.1 A brief history of polarons

The concept of a polaron can be traced back to the seminal paper by Landau nearly a century ago [1] in which he imagines the internal dynamics in a crystal from the point of view of a single electron. As the electron moves through an ionic crystal it naturally induces disturbances in the lattice as visualized in Figure 1.1, which can be thought of as a polarization cloud following the electron. It turns out to be useful to think of the electron together with all the disturbances in the lattice as a single quasiparticle – later appropriately coined as the *polaron* by Pekar [2]. The polaron has a number of interesting properties different from the bare electron, such as a binding energy, effective mass or radius. If the polaron is small enough, discrete lattice properties have to be taken into account described by the Holstein polaron model [3], but in general we will be concerned with large polarons in a continuous description. An important generalization that allowed to study these properties more rigorously was a formulation of the problem in the language of a many-body Hamiltonian in second quantization in the Fröhlich model [4]. Herein the electron is described as an impurity interacting with a quantum field of excitations which represent the phonons of the lattice, a picture still used to this day. Not long after the onset of these theoretic predictions the first polaronic

effects were observed in an experiment [5].



FIGURE 1.1: A visual depiction of the electron disturbing the ionic lattice (left) and and impurity disturbing the particles in a Bose gas (right). Courtesy of APS/Carin Cain; Physics 9, 86 (2016).

Although the Fröhlich model turns out to be suitable to describe large polarons, the problem of theoretically studying a many-body quantum system is far from easy and strongly depends on the system-specific properties. The first attempt to crack open the problem was made by Pekar [2], relying on a classical product ansatz in which the electron is strongly localized. At the time it was well known that this approximation works well in the limit of strong coupling between the impurity and phonons, but only recently a rigorous proof has been formulated [6]. The other seminal approach in the literature is the Lee Low Pines approach [7], where the crucial step can be thought of as an inverse Hubbard-Stratonovic transformation. In this approach the electron is integrated out, and one remains with a phonon field which now exhibits difficult quartic interactions that are mediated by the electron. A mean-field approximation of this effective field yields a description which is valid at weaker coupling.

The significant breakthrough that provided the all-coupling approach was formulated by Feynman [8], which is perhaps the most illustrative case in nonrelativistic physics where the path integral approach yields a superior solution. In this paper, the complicated polaron system of an electron and phonons described by the Fröhlich model is mapped on a simple coupled harmonic oscillator model for which then a variational criterion is formulated in the path integral approach. In the semi-analytical realm, the approach is to this day arguably considered the most successful principle due to its simplicity and remarkable accuracy for large solid state polarons coupling to either the optical or acoustic phonons [9, 10]. In the decades to follow numerous new theoretical investigations and experimental results for polarons in materials have been obtained, which the interested reader can find in the recent review [11].

The scope of polaronic physics has since then been significantly broadened to the study of impurities interacting with excitations of some medium in which they are immersed. For example, in (anti)ferromagnetic solids the charge carriers or holes could mainly be coupled to magnetic excitations of the lattice instead of the phonons, resulting in the *spin polaron* [12]. On the other hand, impurities can still be electrons but on a completely different medium such as for example liquid helium films [13] forming the *ripplopolarons*. As a final example, instead of electrons, quasiparticles such as bound electron-hole pairs could be coupling to the phonons, which form the class of exciton-polarons [14].

More recently, a new class of polarons in ultracold atomic quantum gases has been the subject of intensive investigation. Here, an atom of a different type or in a different spin state is immersed into either a Fermi gas or a Bose gas and exhibits a polaronic effect due to disturbing the gas as shown in Figure 1.1. The first type of experimental realizations concerned observing polaronic effects of impurities in degenerate Fermi gases [15–18]. From an experimental point of view Fermi gases were more accessible in initial studies due to the absence of inelastic three-body collisions and a greater spatial extent [19]. For this reason it took longer to realize the Bose polaron counterpart. Following upon a series of experimental improvements [20–22], finally in 2016 two parallel experiments at JILA and Aarhus have presented observations of Bose polarons up to the strong coupling regime [19, 23]. More advanced experimental studies followed later, such as probing the Bose polaron at criticality [24] or an investigation of the dynamics of Bose polaron formation [25]. Even in the absence of impurities, Bose-Einstein condensates are delicate systems and it is illustrative to first discuss them separately in the next section.

1.2 Bose-Einstein condensation

1.2.1 IDENTICAL PARTICLES

Imagine two identically looking apples, or other fruit of choice, placed on a table in front of you and then get cautiously interchanged in front of your eyes. As far

as you can tell the apples have no markings or other traces to tell them apart, and to the best of your knowledge the setup looks identical as before. Yet if you were asked the somewhat absurd question "Is the universe the same as before?" it is not unlikely that your basic intuition would tell you that something has changed and the two cases are somehow still distinct realizations of all the possible states of the world. This is quite reasonable, and sometimes you can get away with this intuition. For example, when describing the apples as classical objects one can study the phase space of positions and momenta $\{\mathbf{r}_1, \mathbf{p}_1, \mathbf{r}_2, \mathbf{p}_2\}$ with each of the labels referring to a specific apple and obtain a perfectly valid classical physics description.

However, at the fundamental level particles can be *truly* identical. When assigning probabilities to finding particles at positions \mathbf{r}_1 and \mathbf{r}_2 , there should be no measurable way to tell one case apart from the other. In the language of quantum mechanics this property is imposed on the quantum state Ψ of a system through:

$$|\Psi(\mathbf{r}_1, \mathbf{r}_2)|^2 = |\Psi(\mathbf{r}_2, \mathbf{r}_1)|^2.$$
(1.1)

Any state Ψ that describes the probability density amplitude of the particles has to be unchanged up to a global phase when the positions of identical particles are exchanged. It turns out that as fundamental particles, only two classes are known to exist: bosons and fermions with an exchange phase of respectively 1 or -1, where the former will be our main focus for now. This innocuous looking restriction has a tremendous impact on the way combinatorics of different particle states is performed, which in turn changes the particle statistics. We will return to this statistical way of looking at the problem in great technical detail later in this thesis, but let us first consider a qualitative discussion of bosons at low temperatures.

1.2.2 Macroscopic ground state

As already alluded to previously, in some circumstances the quantum mechanical or identical nature of particles can be completely ignored while in others it becomes of crucial importance. The argument found in many textbooks on thermal physics e.g. [26, 27] nicely captures a qualitative picture of the transition from a classical to a quantum regime. Consider the case of a gas of N particles of mass m trapped in a box of volume V at a temperature T. The typical length scale at which individual particles in the gas exhibit quantum mechanical wavelike properties can be estimated by the thermal de Broglie wavelength [26]:

$$\lambda_{\rm th} = \sqrt{\frac{2\pi\hbar^2}{mk_B T}},\tag{1.2}$$

where \hbar is the reduced Planck constant and k_B the Boltzmann constant. When this scale is far smaller than the average interparticle distance $\lambda_{\rm th} \ll (V/N)^{1/3}$ on average the particles do not feel each other's wavelike nature and hence the gas behaves as a classical system of point particles. As can be seen from (1.2) this is typically the case when either the temperature is sufficiently high or when the gas is sufficiently dilute. On the other hand, as the gas is cooled at some critical temperature T_c the length scales become comparable and $\lambda_{\rm th} \approx (V/N)^{1/3}$. As the particle waves start to overlap in this regime the quantum effects become dominant and a bosonic system forms a composite macroscopic matter wave as depicted in Figure 1.2. Roughly speaking, in this regime the distinction between separate particles is completely lost and the system behaves as a single quantum mechanical wave packet forming the *Bose-Einstein condensate* (BEC).



FIGURE 1.2: As the temperature is decreased the quantum wavelike properties of the particles start to overlap and the gas forms a macroscopic wave. Figure adapted from [27], with the permission of Springer Nature.

In 1995 at JILA [28] a gas of ⁸⁷Rb atoms was cooled to temperatures of ~ 170nK at which observations of velocity profiles for the first time ever confirmed the existence of a BEC, not much later followed by similar observations in experiments at MIT [29] in gases of ¹¹Na atoms. Similar experiments were being performed at Rice, using ⁷Li atoms [30]. For these groundbreaking observations the 2001 Nobel Prize in physics was awarded to E. Cornell, C. Wieman (from the JILA experiment) and W. Ketterle (from the MIT experiment). The experimental details of how

BECs are created and captured in typical experiments will be discussed in more depth further on when discussing Bose polarons.

1.2.3 Bogoliubov Theory

The theoretical description of a Bose gas at low temperatures forms a great challenge and has been the subject of intense theoretical study for many decades now. Roughly speaking, the challenge lies in simultaneously capturing non-quadratic interactions between the particles, quantum fluctuations of the system, and identical particle statistics at non-zero temperature. Before proceeding to a discussion of the method of choice, a few notable approaches should be mentioned. When the temperature is assumed to be zero and quantum fluctuations are ignored but interactions can be arbitrarily strong, the system is well described by the Gross-Pitaevskii equation [31, 32]. On the other hand, if interactions are assumed to be weak but quantum fluctuations are to be captured exactly, perturbative approaches allow one to find corrections to the ground state [33]. Also note that even when interactions are completely absent, describing a fixed number of bosons at non-zero temperatures while correctly taking the identical nature into account forms a difficult statistical problem [34, 35]. Finally, Monte Carlo methods can be used to compute exact quantities of the system, but of course require far greater computational resources and yield less physical transparency [36]. One approach to the problem that conceptually lies somewhere between the Gross-Pitaevskii equation and perturbation theory is Bogoliubov theory [37, 38]. In this approach a perturbative expansion is performed around the macroscopically occupied ground state of the gas, which implicitly assumes the temperature to be near-zero and the interactions to be weak. Since Bogoliubov theory will be the framework of choice through which a Bose gas will be viewed in this thesis, a brief summary is presented below.

Consider a free interacting gas of bosonic particles with mass m_b , in a box of volume V, described in second quantization by the creation and annihiliation operators $\hat{a}^{\dagger}_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}$ that create or annihilate a boson with momentum $\hbar \mathbf{k}$. The Hamiltonian of the system is then given by:

$$\hat{H}_{BEC} = \sum_{\mathbf{k}} E_{\mathbf{k}} \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{q}} V_{\mathbf{q}}^{(BB)} \sum_{\mathbf{k},\mathbf{k}'} \hat{a}_{\mathbf{k}+\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{k}'-\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{k}'} \hat{a}_{\mathbf{k}}.$$
(1.3)

The first term describes the kinetic energy of the system with energy spectrum

1.2 - Bose-Einstein condensation

 $E_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m_b}$, and the second term represents the interaction part where $V_{\mathbf{q}}^{(BB)}$ is the boson-boson interaction amplitude in momentum space. In the rest of this thesis the interaction between the bosons will be considered to be a contact interaction for which the amplitude is set equal to a coupling constant $V_{\mathbf{q}}^{(BB)} = g_{bb}/V$.

The trick now is to realize that if the ground state of the condensate is macroscopically occupied, the operators that correspond to the $\mathbf{k} = 0$ mode provide the dominant contribution. The interaction contributions to the Hamiltonian can now be expanded in terms of their order in the \hat{a}_0 operators. The Bogoliubov approximation consists out of two steps. First, the terms of zeroth and first order in \hat{a}_0 are discarded as they will be small in comparison to the higher order contributions:

$$\hat{H}_{BEC} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m_b} \hat{a}^{\dagger}_{\mathbf{k}} \hat{a}_{\mathbf{k}} + \frac{g_{bb}}{2V} \hat{a}^{\dagger}_0 \hat{a}^{\dagger}_0 \hat{a}_0 \hat{a}_0 + \frac{g_{bb}}{2V} \sum_{\mathbf{k} \neq 0} \left(4 \hat{a}^{\dagger}_0 \hat{a}^{\dagger}_{\mathbf{k}} \hat{a}_{\mathbf{k}} \hat{a}_0 + \hat{a}^{\dagger}_{\mathbf{k}} \hat{a}^{\dagger}_{-\mathbf{k}} \hat{a}_0 \hat{a}_0 + \hat{a}^{\dagger}_0 \hat{a}^{\dagger}_0 \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} \right).$$
(1.4)

Next, a mean field approximation of the ground state operators is made $\hat{a}_0 = \hat{a}_0^{\dagger} = \sqrt{N_0}$, where N_0 is the number of atoms in the ground state. The fourth order term is typically rewritten as:

$$\hat{a}_{0}^{\dagger}\hat{a}_{0}^{\dagger}\hat{a}_{0}\hat{a}_{0} = \left(N - \sum_{\mathbf{k}\neq0}\hat{a}_{\mathbf{k}}^{\dagger}\hat{a}_{\mathbf{k}}\right)\left(N - \sum_{\mathbf{k}\neq0}\hat{a}_{\mathbf{k}}^{\dagger}\hat{a}_{\mathbf{k}}\right) \approx N^{2} - 2\sum_{\mathbf{k}\neq0}\hat{a}_{\mathbf{k}}^{\dagger}\hat{a}_{\mathbf{k}},\qquad(1.5)$$

where N is the total number of bosons. In the Bogoliubov approximation the Hamiltonian becomes:

$$\hat{H}_{BEC} = \frac{g_{bb}N^2}{2V} + \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m_b} \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} + \frac{g_{bb}n_0}{2} \sum_{\mathbf{k}\neq 0} \left(2\hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} + \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{-\mathbf{k}}^{\dagger} + \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} \right), \quad (1.6)$$

where n_0 is the density of the bosons in the ground state. The first term is the BEC mean-field energy term that represents the energy of the fully condensed Bose gas at T = 0, whereas the other terms capture the corrections from excitations caused by interactions. The Hamiltonian is now completely quadratic in the operators and can be diagonalized in a final step through the Bogoliubov transformation:

$$\hat{a}_{\mathbf{k}}^{\dagger} = \left(u_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} + v_{-\mathbf{k}} \hat{\alpha}_{-\mathbf{k}} \right), \qquad (1.7)$$

$$\hat{a}_{\mathbf{k}} = \left(u_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} + v_{-\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}^{\dagger} \right), \qquad (1.8)$$

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where the condition $|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1$ imposes that the operators $\hat{\alpha}$ also obey bosonic commutation relations. The parameters $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ can now be chosen appropriately:

$$u_{\mathbf{k}} = \left[\frac{\frac{\hbar^2 k^2}{2m_b} + g_{bb} n_0}{2\hbar\omega_{\mathbf{k}}} + \frac{1}{2}\right]^{1/2},$$
(1.9)

$$v_{\mathbf{k}} = \left[\frac{\frac{\hbar^2 k^2}{2m_b} + g_{bb} n_0}{2\hbar\omega_{\mathbf{k}}} - \frac{1}{2}\right]^{1/2},\tag{1.10}$$

such that in the new basis the Hamiltonian is diagonal:

$$\hat{H}_{BEC} = \frac{g_{bb}N^2}{2V} + \frac{1}{2}\sum_{\mathbf{k}\neq 0} \left(\hbar\omega_{\mathbf{k}} - g_{bb}n_0 - \frac{\hbar^2 k^2}{2m_b} + \frac{m_b g_{bb}^2 n_0^2}{\hbar^2 k^2} \right) + \sum_{\mathbf{k}\neq 0} \hbar\omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}}$$
$$= E_0^{(BEC)} + \sum_{\mathbf{k}\neq 0} \hbar\omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}}.$$
(1.11)

This is the Bogoliubov Hamiltonian which on top of the corrected ground state energy yields an excitation spectrum of Bogoliubov quasiparticles with energy spectrum:

$$\hbar\omega_{\mathbf{k}} = \sqrt{\frac{\hbar^2 k^2}{2m_b} \left(\frac{\hbar^2 k^2}{2m_b} + 2g_{bb} n_0\right)}.$$
(1.12)

In an undisturbed Bose gas at T = 0 all the quasiparticles are in the so called Bogoliubov vacuum corresponding to $\mathbf{k} = 0$ state, and hence the energy is given by $E_0^{(BEC)}$. An increase in temperature or a disturbance of the Bose gas will then create excitations in the Bose gas which can be easily described in this framework. The low energy spectrum $\omega_{\mathbf{k}} \sim k$ yields collective excitations that are sometimes called the phonons of the gas, whereas at high energies $\omega_{\mathbf{k}} \sim k^2$ the excitations are particle like and represent condensed atoms getting expelled out of the condensate. Note that an important length scale can be associated with the energy of crossover $\hbar^2/(m_b\xi^2) = 2g_{bb}n_0$ in 1.12, which is defined as the healing length of the condensate $\xi = \sqrt{\hbar^2/(2mg_{bb}n_0)}$.

When an impurity is immersed into a Bose gas it creates a cloud of excitations surrounding itself forming the Bose polaron. Bogoliubov theory therefore provides a perfect analogy with the solid state polaron where the electron is interacting with excitations of the lattice – the phonons. Before proceeding further with this discussion let us first summarize a few experimental aspects of how Bose polarons are created. The discussion will mainly concern the Aarhus experiment where the impurities themselves are bosonic. For all practical purposes of this thesis, the JILA experiment studies similar quantities and the main difference is that the impurities are fermions.

1.3 Observations of Bose polarons at Aarhus

In this section we provide a brief summary of the seminal experiment at Aarhus [23]. The Aarhus experiment starts out by creating a BEC of 39 K atoms in the $|1\rangle = |1, -1\rangle$ hyperfine state trapped in an optical dipole trap. This apparatus is capable of trapping a cloud of neutral atoms in the minimum of its intensity field. The basic principle is that the laser light induces a dipole moment in each of the atoms, which then interacts with the gradient of the intensity of the laser light creating a trapping force. For a more comprehensive discussion of this trapping mechanism a review can be found in [39]. The trap therefore effectively creates a harmonic trapping potential for the atoms with the following anisotropic trapping frequencies in the experiment $\nu_x = 158$ Hz, $\nu_y = 167$ Hz and $\nu_z = 228$ Hz. The average density of the condensate is given by $n_0 = 2.3 \times 10^{14} \text{cm}^{-3}$ and the temperature is estimated to be T = 160 nK. Although the temperature is well below the critical temperature, $T \approx 0.6T_c$, such that the bosons are condensed, it is not quite in the $T \ll T_c$ regime and it is important to keep in mind that thermal fluctuations could be of importance for a quantitative comparison. Nevertheless, as will be argued in the next chapter, the description of the Bose polaron is theoretically extremely challenging due to large quantum fluctuations and for this reason many studies in the past years have focused on the T = 0 regime.

Next, the impurities in the experiment are created by transferring a fraction of the $|1\rangle$ atoms into a different hyperfine state $|2\rangle = |1,0\rangle$ by shining a square radiofrequency pulse of $100\mu s$ at a frequency ω_{RF} . The $|2\rangle$ states are the impurities of the polaron problem, forming a minority fraction in a majority of $|1\rangle$ condensed atoms. The interactions between the two states can be described as s-wave contact interactions with a scattering length a_{ib} , which can be tuned in the experiment through the phenomenon of Feshbach resonances [40].

To understand the meaning of this parameter it is illustrative to think of the scattering of the impurity on a box-potential with the same scattering length, which is in detail described in numerous quantum mechanics textbooks e.g. [41]. When the box is extremely shallow, a_{ib} is small and negative and corresponds with

effective attractive interactions, but as the depth of the box increases, a_{ib} keeps growing in the negative direction. At some point the box becomes sufficiently deep to support a shallow bound state which is exactly the $a_{ib} \rightarrow -\infty$ limit. From this point onwards, there is always an available molecular ground state (where the impurities form tightly bound molecules with the rest of the atoms). However when the formation of the molecule is energetically prohibited, the particle experiences a strong effective repulsion corresponding to the $a_{ib} \rightarrow +\infty$ limit. Increasing the box depth further moves the shallow bound state deeper and decreases the effectively repulsive interactions in the limit of $a_{ib} \rightarrow 0^+$. Accordingly, for $a_{ib} > 0$ in the experimental measurements, as shown in Figure 1.3, two branches can be recognized, one corresponding to the state created by repulsive interactions and the other to the molecular branch where the bosons get tightly bound to the impurities. In the rest of the thesis we will largely, but not solely, be concerned with the repulsive branch that gets measured in the experiments. As can also been seen from this discussion it is more useful to use a_{ib}^{-1} as a scaling parameter which is precisely done in the experimental studies. By tuning this parameter, the experimental setup therefore provides for the perfect ground to study the properties of the impurity across an entire range of interaction regimes.



FIGURE 1.3: The Bose polaron spectroscopy measurements from the Aarhus experiment. The experimentally measured spectroscopy signal (a) and theoretical calculations of the truncated basis method (b). The three polaronic branches, attractive – bottom left, repulsive – top right, molecular – bottom right, can be clearly distinguished. Figure adapted from [23], with the permission of the American Physical Society.

In the presence of magnetic fields, the $|1\rangle \rightarrow |2\rangle$ transition has a corresponding bare frequency ω_0 . Therefore, even in the absence of interactions between the

states, a spectroscopy measurement in the RF domain yields a peak centered at ω_0 with a finite width due to the short pulse duration. In the presence of interactions, the experiment is repeated and a shift of the peak is observed towards a frequency ω . The shift $\Delta = \omega - \omega_0$ is therefore evidence of a dressing of the impurity, and represents the energy of the Bose polaron. The full spectroscopy results at Aarhus are shown in Figure 1.3 as a function of the inverse scattering length where the color map represents the spectroscopic signal. We can easily recognize two main branches which we will refer to as the attractive or repulsive polaron branches. In addition, a third branch can be recognized corresponding to the molecular bound state of the impurity and a boson. The attractive polaron has a negative energy shift indicating a stable state that transitions into molecular bound states as a_{ib} crosses to the positive domain. Numerous recent studies have discussed the attractive branch [42-45] in great detail, where it was shown that the Efimov effect is of crucial importance to correctly describe the bound states in this regime. The repulsive branch has a positive energy shift and is therefore metastable. The impurities want to be expelled out of the condensate and as can be seen from the figure could also decay into the lower lying molecular states. Nevertheless, the repulsive polaron lies much closer to the original polaron concept than the molecular state of the attractive branch. The impurity does not bind to one of the bosons and remains completely free to scatter of the phonons forming a difficult many-body problem. In this thesis, mainly methods capable of correctly capturing the repulsive branch will be discussed.

By fitting the center of the peaks observed in Figure 1.3 the experiments are able to present a definite value of the polaron ground state energy as a function of the interaction strength. While the experimental setup at the JILA experiment [19] is quite different, they present measurements of similar results for the Bose polaron energy in a heteronuclear gas of atoms. Also note that since the original publication [23], a new analysis of the Aarhus experiment by taking into account the inhomogeneity of the trap has slightly modified the values for the energy [46].

1.4 Theoretical models for Bose polarons

1.4.1 The Bogoliubov-Fröhlich Hamiltonian

Having obtained an idea of how Bose polarons are created in experiments, let us proceed to introduce a theoretical model and its various simplifications. The

model described here was first introduced for the Bose polaron [47, 48], and has since then featured in numerous works which will be discussed more closely in the next chapter. The Hamiltonian for N_I impurities with masses m described by first quantization operators for the momenta $\hat{\mathbf{p}}_i$ and positions $\hat{\mathbf{r}}_i$ interacting with a Bose gas through contact interactions with strength g_{ib} is written as:

$$\hat{H} = \hat{H}_{imp} + \hat{H}_{BEC} + \hat{H}_{int} = \sum_{\mathbf{j}}^{N_I} \frac{\hat{\mathbf{p}}_j^2}{2m} + \frac{1}{2} \sum_{i \neq j}^{N_I} U(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j) + \sum_{\mathbf{k}} E_{\mathbf{k}} \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{q}} V_{\mathbf{q}}^{BB} \sum_{\mathbf{k},\mathbf{k}'} \hat{a}_{\mathbf{k}+\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{k}'-\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{k}'} \hat{a}_{\mathbf{k}} + \sum_{\mathbf{q}} V_{\mathbf{q}}^{IB} \hat{\rho}_{\mathbf{q}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}-\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{k}}.$$
(1.13)

The first two terms describe the impurities interacting between one another through some direct interaction potential $U(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j)$. Since in the experiment this interaction is small in comparison with the typical impurity-boson interaction strength, most often this term will be discarded. The third and fourth terms are nothing else than the Bose gas Hamiltonian (1.3) with contact interactions, discussed in Sec. 1.2.3. Finally, the last term describes how the bosons in the gas can scatter off the impurity density

$$\hat{\rho}_{\mathbf{q}} = \sum_{j=1}^{N_I} e^{i\mathbf{q}\cdot\hat{\mathbf{r}}_j}.$$
(1.14)

Just like for the boson intraspecies interactions, we assume contact interactions such that $V_{\mathbf{q}}^{(IB)} = g_{ib}/V$, where g_{ib} is the contact interaction strength between the impurities and the Bose gas. The problem one faces now is that the full Hamiltonian (1.13) is quite difficult, even in the absence of impurities.

For this reason, to obtain an approximate Hamiltonian in the regime of small BEC depletion, the Bogoliubov approximation and transformation discussed in Sec. (1.2.3) is performed on this Hamiltonian. For the first two terms of Hamiltonian (1.13) this yields the following expression:

$$\hat{H}_{BEC} + \hat{H}_{imp} = E_0^{(BEC)} + \sum_{\mathbf{k}\neq 0} \hbar \omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \sum_{\mathbf{j}}^{N_I} \frac{\hat{\mathbf{p}}_j^2}{2m}, \qquad (1.15)$$

where $\hat{\alpha}_{\mathbf{k}}^{\dagger}$, $\hat{\alpha}_{\mathbf{k}}$ are the Bogoliubov operators of the previous section. The interaction part \hat{H}_{int} can also be taken into account within Bogoliubov theory. Let us start by dividing the interaction part of the Hamiltonian in terms that couple to the

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condensate in second, first and zeroth order:

$$\hat{H}_{\text{int}} = \frac{g_{ib}}{V} \hat{a}_{\mathbf{0}}^{\dagger} \hat{a}_{\mathbf{0}} + \frac{g_{ib}}{V} \sum_{\mathbf{q}\neq\mathbf{0}} \hat{\rho}_{\mathbf{q}} \left(\hat{a}_{\mathbf{0}}^{\dagger} \hat{a}_{\mathbf{q}} + \hat{a}_{-\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{0}} \right) + \frac{g_{ib}}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \sum_{\mathbf{q}\neq\mathbf{k}} \hat{\rho}_{\mathbf{q}} \hat{a}_{\mathbf{k}-\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{k}}.$$
 (1.16)

In what follows we perform the Bogoliubov approximation to obtain $\hat{a}_{\mathbf{0}}^{\dagger} = \hat{a}_{\mathbf{0}} \approx \sqrt{N_0}$:

$$\hat{H}_{\text{int}} = g_{ib}n_0 + \frac{g_{ib}\sqrt{N_0}}{V} \sum_{\mathbf{q}\neq\mathbf{0}} \hat{\rho}_{\mathbf{q}} \left(\hat{a}_{\mathbf{q}} + \hat{a}_{-\mathbf{q}}^{\dagger}\right) + \frac{g_{ib}}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \sum_{\mathbf{q}\neq\mathbf{k}} \hat{\rho}_{\mathbf{q}} \hat{a}_{\mathbf{k}-\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{k}}, \qquad (1.17)$$

where n_0 is the condensate density. First, let us consider the case where the interactions between the impurity and the condensate are very weak such that the presence of the impurity does not create too many excitations in the gas. In this case the higher order terms in (1.17) can be discarded since they only involve processes with particles out of the condensate. Performing the Bogoliubov transformations (1.7) and (1.8) on the operators in the round brackets yields:

$$\hat{H}_{\text{int}} = g_{ib}n_0 + \frac{g_{ib}\sqrt{N_0}}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \hat{\rho}_{\mathbf{k}} \left((u_k + v_k)\hat{\alpha}_{\mathbf{k}} + (u_{-k} + v_{-k})\hat{\alpha}_{-\mathbf{k}}^{\dagger} \right).$$
(1.18)

Using the previously introduced parameters u_k and v_k in (1.9) and (1.10) it is not difficult to show that

$$V_{\mathbf{k}} = u_{\mathbf{k}} + v_{\mathbf{k}} = \left(\frac{\frac{\hbar^2 k^2}{2m_b}}{\frac{\hbar^2 k^2}{2m_b} + 2g_{bb}n_0}\right)^{1/4}.$$
 (1.19)

With this result we can now write down the full Hamiltonian:

$$\hat{H} \approx E_0^{(BEC)} + g_{ib}n_0 + \sum_{\mathbf{j}}^{N_I} \frac{\hat{\mathbf{p}}_j^2}{2m} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{g_{ib}\sqrt{N_0}}{V} \sum_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{-\mathbf{k}}^{\dagger} \right).$$
(1.20)

The three terms on top of the constant energy shift in (1.20) form nothing else than the seminal Fröhlich Hamiltonian [4]. To specify that the dispersion relation and interaction amplitude are to be chosen for the Bose gas as a medium, this model is also called the Bogoliubov-Fröhlich Hamiltonian:

$$\hat{H}_F = \sum_{\mathbf{j}}^{N_I} \frac{\hat{\mathbf{p}}_j^2}{2m} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{g_{ib}\sqrt{N_0}}{V} \sum_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{-\mathbf{k}}^{\dagger} \right)$$
(1.21)

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This Hamiltonian describes N_I impurities with some many-body density operator $\rho_{\mathbf{k}}$ interacting with the Bogoliubov excitations of the BEC with dispersion relation $\omega_{\mathbf{k}}$. The last term describes the simplest possible interaction between the systems, where the impurities can either create or absorb excitations in the condensate with an amplitude $\sim g_{ib}V_{\mathbf{k}}$. One should not be deceived by the simplicity of this Hamiltonian. Although the interaction term can be written compactly in this form, remember that the impurity density operator (1.14) is of second order in the impurity operators when written in second quantization. The Hamiltonian therefore describes a many-body problem to *third order* and has no known analytic solution.

1.4.2 The extended Fröhlich Hamiltonian

In the previous subsection we have discarded the higher order terms in expression (1.17) to obtain the Fröhlich Hamiltonian. As emphasized, this step relies on the fact that the number of excited atoms is sufficiently small to only take the impurity kicking atoms out of the ground state (or returning them) into account. As the coupling strength g_{ib} becomes larger, higher order interactions where the impurity is interacting with the excited cloud it created can no longer be neglected. This direction has been first explored in [49] and the extended-Fröhlich Hamiltonian presented further was first explored at the mean-field dynamics level in [50]. If the final term of (1.17) is taken into account as well, one obtains on top of the Fröhlich Hamiltonian the following extended interaction terms:

$$\frac{g_{ib}}{V} \sum_{\mathbf{s}\neq\mathbf{0}} \sum_{\mathbf{k}\neq\mathbf{0}} \hat{\rho}_{\mathbf{k}-\mathbf{s}} W_{\mathbf{k},\mathbf{s}}^{(1)} \hat{\alpha}_{\mathbf{s}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{1}{2} \frac{g_{ib}}{V} \sum_{\mathbf{s}\neq\mathbf{0}} \sum_{\mathbf{k}\neq\mathbf{0}} \hat{\rho}_{\mathbf{k}-\mathbf{s}} W_{\mathbf{k},\mathbf{s}}^{(2)} \left(\hat{\alpha}_{\mathbf{s}}^{\dagger} \hat{\alpha}_{-\mathbf{k}}^{\dagger} + \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{-\mathbf{s}} \right) \\
+ \frac{g_{ib}}{V} N_{I} \sum_{\mathbf{k}\neq\mathbf{0}} v_{\mathbf{k}}^{2} \tag{1.22}$$

The first term of this interaction part describes a phonon from the excitation cloud scattering off an impurity and exchanging a momentum $\mathbf{k} - \mathbf{s}$. The second term describes an impurity either creating or absorbing two phonons from the excitation cloud hereby also absorbing momentum $\mathbf{k} - \mathbf{s}$. The amplitudes for the two types of processes are given by respectively:

$$W_{\mathbf{k},\mathbf{k}'}^{(1)} = \frac{1}{2} \left(V_{\mathbf{k}} V_{\mathbf{k}'} + V_{\mathbf{k}}^{-1} V_{\mathbf{k}'}^{-1} \right), \qquad (1.23)$$

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$$W_{\mathbf{k},\mathbf{k}'}^{(2)} = \frac{1}{2} \left(V_{\mathbf{k}} V_{\mathbf{k}'} - V_{\mathbf{k}}^{-1} V_{\mathbf{k}'}^{-1} \right).$$
(1.24)

The summation in the final term over the Bogoliubov coefficient $\sum_{\mathbf{k}} v_{\mathbf{k}}^2$ can be shown to be equal to the number of excited bosons within Bogoliubov theory $n_{\text{bog}}^{(\text{exc.})}$ in the absence of the impurity. Taking the boson operators into account up to second order in the impurity-condensate interaction term (1.16) therefore also yields a correction to the mean field term $g_{ib}n_0$. Combining everything we obtain for the full Bose polaron Hamiltonian:

$$\hat{H} \approx g_{ib} \left(n_0 + n_{\text{bog}}^{(\text{exc.})} \right) + \sum_{\mathbf{j}}^{N_I} \frac{\hat{\mathbf{p}}_j^2}{2m} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{g_{ib} \sqrt{N_0}}{V} \sum_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{-\mathbf{k}}^{\dagger} \right) + \frac{g_{ib}}{V} \sum_{\mathbf{s} \neq \mathbf{0}} \sum_{\mathbf{k} \neq \mathbf{0}} \hat{\rho}_{\mathbf{k}-\mathbf{s}} W_{\mathbf{k},\mathbf{s}}^{(1)} \hat{\alpha}_{\mathbf{s}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{1}{2} \frac{g_{ib}}{V} \sum_{\mathbf{s} \neq \mathbf{0}} \sum_{\mathbf{k} \neq \mathbf{0}} \hat{\rho}_{\mathbf{k}-\mathbf{s}} W_{\mathbf{k},\mathbf{s}}^{(2)} \left(\hat{\alpha}_{\mathbf{s}}^{\dagger} \hat{\alpha}_{-\mathbf{k}}^{\dagger} + \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{-\mathbf{s}} \right),$$

$$(1.25)$$

where we will measure the energy relative to $E_0^{(BEC)}$. Note that in general $n_{\text{bog}}^{(\text{exc.})}$ is extremely small for weakly interacting Bose gases in three dimensions, and within the confines of Bogoliubov theory we will just keep $g_{ib}n_0$ as the mean field energy term. Just as for the Fröhlich Hamiltonian, the contribution on top of the mean-field shift can be defined as the extended-Fröhlich Hamiltonian:

$$\hat{H}_{EF} = \sum_{\mathbf{j}}^{N_{I}} \frac{\hat{\mathbf{p}}_{j}^{2}}{2m} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{g_{ib}\sqrt{N_{0}}}{V} \sum_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{-\mathbf{k}}^{\dagger} \right) + \frac{g_{ib}}{V} \sum_{\mathbf{s}\neq\mathbf{0}} \sum_{\mathbf{k}\neq\mathbf{0}} \hat{\rho}_{\mathbf{k}-\mathbf{s}} W_{\mathbf{k},\mathbf{s}}^{(1)} \hat{\alpha}_{\mathbf{s}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{1}{2} \frac{g_{ib}}{V} \sum_{\mathbf{s}\neq\mathbf{0}} \sum_{\mathbf{k}\neq\mathbf{0}} \hat{\rho}_{\mathbf{k}-\mathbf{s}} W_{\mathbf{k},\mathbf{s}}^{(2)} \left(\hat{\alpha}_{\mathbf{s}}^{\dagger} \hat{\alpha}_{-\mathbf{k}}^{\dagger} + \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{-\mathbf{s}} \right).$$

$$(1.26)$$

It is important to remember that this Hamiltonian is still situated within the confines of Bogoliubov theory for the condensate, and the number of excited atoms is assumed to be small. However, the extended Fröhlich Hamiltonian provides the first correction to also account for the interactions between the impurity and the excited atoms.

1.4.3 Full Bose polaron energy

The approximate Hamiltonian is now written as:

$$\hat{H} \approx E_0^{(BEC)} + g_{ib}n_0 + \hat{H}_F,$$
 (1.27)

where \hat{H}_F should be replaced by \hat{H}_{EF} for the extended Fröhlich model, but the rest of the discussion holds for both models. As long as the Bogoliubov approximation is valid and n_0 is constant, the BEC intraspecies interaction energy is not influenced by the presence of the impurity and the Bose polaron energy can be measured with respect to $E_0^{(BEC)}$. One slightly awkward feature of this system is that by defining the Fröhlich Hamiltonian as (1.21) to make the connection with other polaronic systems, one is left with the energy shift $g_{ib}n_0$ that does depend on the impurity interaction strength, but is not incorporated in the Hamiltonian of interest. From an experimental point of view, it is of course interesting to measure the energy with respect to $g_{ib} = 0$, while for theoretical work it is convenient to discard this term and study the energy scales of the Fröhlich Hamiltonian (1.21) directly. In addition, the mean-field impurity-condensate interaction energy $q_{ib}n_0$ is not particularly interesting in that it merely represents the energy contribution of the physical situation where the impurity is completely delocalized and not influenced by the condensate in any shape or form and hence does not arise from polaronic effects. For this reason, often the *polaronic contribution* to the energy E_p is defined as the energy arising from \hat{H}_F such that the energy of the impurity in the condensate is written as:

$$E = g_{ib}n_0 + E_p \tag{1.28}$$

There is an additional practical reason for why this distinction is useful. For a wide range of interaction strengths the relatively trivial $g_{ib}n_0$ term is much larger than the more challenging E_p . It follows that when comparing different theoretical approaches between one another to gauge their accuracy it could be misleading to compare the full energy. Even approaches that completely fail to describe the impurity-phonon many body state will look reasonably accurate in such a comparison. In fact, if one completely discards any interactions between the impurity and $E_p \approx 0$, a reasonable agreement with experiment [19, 23] at weak to intermediate coupling can still be obtained. This does however not at all mean that the quantum state of the system described by the Fröhlich Hamiltonian is close to that of a decoupled impurity and a condensate, but rather that the energy is a difficult experimental metric to probe the more intricate physics of the problem. To obtain other properties such as the effective mass or radius of the Bose polaron, an accurate description of the polaronic effects is required, which have as of this moment not yet been experimentally measured. Therefore, in the rest of this work, most often the polaronic energy E_p will be used in discussions and figures.

1.4.4 Other Fröhlich Hamiltonians

In the previous parts we have defined the Hamiltonian with the Bose polaron problem in mind from the start. However since in the following discussions we will often be referring to the original Fröhlich model, it can be illustrative to briefly discuss the differences between various Fröhlich models that have been studied. For this purpose let us use a general definition for the Fröhlich Hamiltonian for a single impurity:

$$\hat{H}_F = \frac{\hat{\mathbf{p}}^2}{2m} + \sum_{\mathbf{k}} \epsilon(\mathbf{k}) \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \sum_{\mathbf{k}} \left(\hat{\rho}_{\mathbf{k}} \tilde{V}_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} + \hat{\rho}_{-\mathbf{k}} \tilde{V}_{\mathbf{k}}^{*} \hat{\alpha}_{\mathbf{k}}^{\dagger} \right)$$
(1.29)

This is the general form of the Fröhlich Hamiltonian, but the dispersion relation $\epsilon(\mathbf{k})$ and the interaction amplitude $\tilde{V}_{\mathbf{k}}$ depend on the specific system. The phonons in the original Fröhlich Hamiltonian are longitudinal optical phonons [4] that are very well approximated by a constant dispersion relation $\epsilon(\mathbf{k}) = \hbar \omega_{\text{LO}}$. The interaction amplitude on the other hand goes slowly to zero at large momenta:

$$\tilde{V}_{\mathbf{k}} = -i\frac{\hbar\omega_{\rm LO}}{k}\sqrt{\frac{4\pi\alpha}{V}} \left(\frac{\hbar}{2m\omega_{\rm LO}}\right)^{1/4} \tag{1.30}$$

where α is the coupling constant between the impurity and phonons which generally depends on the material. Although the interaction amplitude is imaginary here, this does not play any significant role as to what type of physics the model describes and the observable quantities come out to be strictly real. This model with this form of dispersion and interaction amplitude has been extensively studied in the literature [51, 52]. One particularly nice feature of having no dispersion relation and a simple $\sim 1/k$ interaction amplitude is that in almost any theoretical treatment of the problem, the momentum dependence of the problem can be integrated out analytically. This will not be possible in models with more difficult forms for $\epsilon(\mathbf{k})$ and $\tilde{V}_{\mathbf{k}}$ which makes numerical computation significantly more difficult.

In most ionic crystals the electrostatic coupling to the LO phonons is dominant which is the reason why the LO phonon Fröhlich model is most commonly studied in the literature. However, the electrons can also be affected by the non-polar vibration of the lattice through its effect on the band structure and hence couple Chapter 1 - Polarons

Dispersion and interaction amplitude of different polaron systems					
	$\epsilon(\mathbf{k})$	$\tilde{V}_{\mathbf{k}}$			
Optical polaron (original Fröhlich)	$\sim \omega_{ m LO}$	$\sim k^{-1}$			
Acoustic polaron	$\sim k$	$\sim \sqrt{k}$			
Ripplopolaron	$\sim k^{\frac{3}{2}}$	$\sim k^{-\frac{1}{2}}$			
BEC polaron (weak coupling)	$\sim \sqrt{k^2(k^2+2)}$	$\sim (k^2/(k^2+2))^{\frac{1}{4}}$			

TABLE 1.1: A few examples of the dispersion relation and interaction amplitude of polaronic systems described by the Fröhlich Hamiltonian.

to the acoustic phonons of the crystal [53]. It turns out that even weak coupling to the acoustic branch has a large effect on self trappig properties of the electron. The polaronic formation caused by coupling to this branch is called the acoustic polaron problem [54], where the dispersion relation of the phonons is unsurprisingly linear $\epsilon(\mathbf{k}) \sim k$ with an interaction amplitude $\tilde{V}_{\mathbf{k}} \sim \sqrt{\alpha k}$. The acoustic polaron model is the first one where the notion of a momentum cutoff Λ becomes of importance since the energy has a UV divergence when taking phonons of arbitrarily large momenta into account. However, this does not form an issue since the phonon momentum in the physical system is limited to the first Brillouin zone, which sets the value of the momentum cutoff.

The Fröhlich model is also encountered in more exotic polaronic systems outside solid state physics. One such example is the ripplopolaron where electrons are pressed against the surface of a liquid helium film by an electric field [55]. The electrons interact with the quantized surface oscillators of the film and form polaronic quasiparticles described by the Fröhlich Hamiltonian with dispersion relation $\epsilon(\mathbf{k}) \sim k^{3/2}$ and interaction amplitude $\tilde{V}_{\mathbf{k}} \sim k^{-1/2}$. Finally of course we have the Bose polaron described by the Fröhlich model at weak coupling derived in the previous section where $\epsilon(\mathbf{k}) \sim \sqrt{k^2(k^2+2)}$ and $V_{\mathbf{k}} \sim \sqrt{k^2/(k^2+2)}$.

In a recent mathematical physics paper that we will return to later on as well, a classification of Fröhlich models is made based on the difficulty of their UV behavior [56]. Briefly summarized, the UV behavior of the Hamiltonian is largely determined by the two norms of the interaction amplitude $a = \int \mathbf{dk} |V_{\mathbf{k}}|^2$ and $b = \int \mathbf{dk} |V_{\mathbf{k}}|^2 / (k^2 + 1)$. As long as one of the two is finite in the limit of $\Lambda \to \infty$ the model remains UV regular. This is the case for both the original Fröhlich model and the ripplopolaron model (in 2D), whereas the acoustic polaron model and Bogoliubov-Fröhlich model fall into the more difficult class of UV divergent Hamiltonians. For the acoustic polaron model this divergence presents no problems since phonons with momenta beyond the Brillouin zone are physically not present in the system. In addition, it turns out that even if this cutoff is taken to infinity, standard theoretical methods are capable of capturing this divergence. As we will discuss in great detail further in this thesis, it will turn out that the Bogoliubov-Fröhlich model on the other hand is the most elusive of all the Fröhlich models mentioned here, as also argued in [56].

1.5 Theoretical methods for polaron physics

In this section we review a number of theoretical tools in the literature to analyze the ground state of the Bose polaron. The discussion will center around the Bogoliubov-Fröhlich Hamiltonian (1.21) for a single impurity which is the simplest case for the purpose of illustration. A nice review containing a thorough discussion of most of these methods applied to the Bose polaron can be found in [57], but for self containment of this thesis we provide a brief overview of the methods relevant for future discussion. Where applicable, we provide references to the extensions of these methods to the extended Fröhlich Hamiltonian (1.26) or to multiple impurites.

1.5.1 Lee Low Pines mean field approach

The Lee Low Pines (LLP) approach has been first introduced for the original Fröhlich problem in 1953 in [7]. The applications of the Lee-Low-Pines approach to the Bose polaron can be found for a single particle in [50, 58] and for multiple particles in [59]. The approach consists out of two steps, the first of which is a completely general *Lee Low Pines transformation* of the Hamiltonian into the impurity frame that also lies at the basis of more advanced approaches, and the second is a mean field approximation in this frame. First, let us note that in the Bogoliubov-Fröhlich Hamiltonian:

$$\hat{H}_F = \frac{\hat{\mathbf{p}}^2}{2m} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}^{\dagger}_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} + \frac{g_{ib}\sqrt{N_0}}{V} \sum_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}^{\dagger}_{-\mathbf{k}} \right)$$
(1.31)

neither the impurity momentum $\hat{\mathbf{p}}$ nor the phonon momentum $\sum_{\mathbf{k}} \hbar \mathbf{k} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}}$ are conserved since $\left[\hat{\mathbf{p}}, \hat{H}_F\right] \neq 0$ and $\left[\sum_{\mathbf{k}} \hbar \mathbf{k} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}}, \hat{H}_F\right] \neq 0$. Unsurprisingly, in the lab frame the impurity and phonon bath can exchange momentum and hence neither

is conserved separately. This can be changed by transforming the Hamiltonian with the following unitary transformation:

$$\hat{U}_{\rm LLP} = \exp\left(i\hat{\mathbf{r}} \cdot \sum_{\mathbf{k}} \mathbf{k} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}}\right)$$
(1.32)

which yields:

$$\hat{H}_{\text{LLP}} = \hat{U}_{\text{LLP}} \hat{H}_F \hat{U}_{\text{LLP}}^{\dagger}$$

$$= \frac{1}{2m} \left(\hat{\mathbf{p}} - \sum_{\mathbf{k}} \hbar \mathbf{k} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} \right)^2 + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{g_{ib} \sqrt{N_0}}{V} \sum_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{-\mathbf{k}}^{\dagger} \right).$$
(1.33)

Note that in this frame, the physical meaning of the momentum operator $\hat{\mathbf{p}}$ changes to that of a total momentum since any eigenstate still has to be transformed back in the lab frame through (1.32). In addition, the Lee Low Pines Hamiltonian (1.33) commutes with the momentum operator $\left[\hat{\mathbf{p}}, \hat{H}_{\text{LLP}}\right] = 0$ and hence for any eigenstate $\hat{\mathbf{p}} \to \mathbf{p}$ is replaced by a c-number. In the simplest case where $\mathbf{p} = 0$, e.g. for the ground state at rest, the Hamiltonian becomes:

$$\hat{H}_{\rm LLP} = \frac{1}{2m} \left(\sum_{\mathbf{k}} \hbar \mathbf{k} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} \right)^2 + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{g_{ib} \sqrt{N_0}}{V} \sum_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{-\mathbf{k}}^{\dagger} \right). \quad (1.34)$$

We can see that the impurity variable has completely disappeared from the problem, at the cost of inducing effective interactions between the excitations at fourth order in (1.34). For this reason the Lee Low Pines transformation is often called a transformation into the frame of the impurity, from the point of view of which the phonons appear to have complicated induced interactions.

The Lee Low Pines Hamiltonian (1.33) is completely general and lies at the basis of more advanced approaches discussed in later subsections of this chapter. The second step of the original Lee Low Pines treatment [7] is to propose a coherent state variational ansatz for the Bogoliubov excitations in the impurity frame:

$$|\alpha\rangle = \exp\left(\sum_{\mathbf{k}} f_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} - f_{\mathbf{k}}^* \hat{\alpha}_{\mathbf{k}}^\dagger\right) |0\rangle, \qquad (1.35)$$

where $|0\rangle$ is the Bogoliubov vacuum. The variational energy of the ground state is

1.5 - Theoretical methods for polaron physics

then written as:

$$E[f_{\mathbf{k}}] = \langle \alpha | \, \hat{H}_{\text{LLP}} \, | \alpha \rangle \,. \tag{1.36}$$

The energy minimum is reached for the following expression for the variational parameters:

$$f_{\mathbf{k}} = -\frac{g_{ib}\sqrt{N_0}}{V} \frac{V_{\mathbf{k}}}{\hbar\omega_k + \frac{\hbar^2k^2}{2m}},\tag{1.37}$$

which yields for the minimal energy:

$$E_{\rm MF} = -\frac{g_{ib}^2 n_0}{V} \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^2}{\hbar \omega_k + \frac{\hbar^2 k^2}{2m}}.$$
 (1.38)

The argument of the summation in (1.38) contains a UV divergence for $|\mathbf{k}| \to \infty$. This is not the first time we will encounter a UV divergence and hence it is useful from this point on to introduce a momentum cutoff Λ as an additional implicit parameter of the Hamiltonian (1.31), in terms of which the divergent part can ad hoc be regularized as follows:

$$E_{\rm MF} = -\frac{g_{ib}^2 n_0}{V} \sum_{\mathbf{k}}^{\Lambda} \frac{V_{\mathbf{k}}^2}{\hbar\omega_k + \frac{\hbar^2 k^2}{2m}} + \frac{g_{ib}^2 n_0}{\hbar^2} \frac{\mu}{\pi^2} \Lambda, \qquad (1.39)$$

where $\mu^{-1} = m^{-1} + m_b^{-1}$ is the reduced mass of the impurity and a boson. A physical justification for the regularization step will be provided in the next subsection.

The power of this approach lies in the fact that the mean-field approximation is made in the impurity frame. It can be easily seen from the transformation (1.32) that the variational ansatz in the lab frame is not simply a product state between the impurity and the phonons and therefore captures some entanglement between the two systems. The phonons on the other hand remain uncorrelated since (1.35) is simply a product ansatz, which is a potential shortcoming of this approach. In the original application to the Fröhlich model [51, 52], this did not turn out to be a significant problem and this treatment yielded excellent results from weak to intermediate coupling and was considered a seminal tool for the study of large polarons in these regimes. As we will see in a later section, in the class of Bogoliubov-Fröhlich model or its extensions, this could not be further from the truth and at large cutoff away from extremely weak coupling the mean field treatment spectacularly fails to capture the polaronic state, forming the first indication of a regime of new physics not present in the original Fröhlich model. Chapter 1 - Polarons

1.5.2 LIPPMANN-SCHWINGER REGULARIZATION

Let us return to (1.39) and justify the regularization procedure on physical grounds. Consider once again the full Bose polaron energy introduced in (1.28) where the polaronic energy is now given by the mean field approach discussed in the previous section:

$$E = g_{ib}n_0 + E_{\rm MF}.$$
 (1.40)

The parameter g_{ib} is the constant in front of the idealized interatomic contact interactions between the impurity and the bosons $g_{ib}\delta(\mathbf{r}_i - \mathbf{r}_b)$ introduced at the very start in the full Hamiltonian (1.13). The relationship between the contact interaction and the physically relevant scattering length a_{ib} is derived through the Lippmann-Schwinger equation and depends on the cutoff [48]:

$$g_{ib}(\Lambda) = \frac{2\pi\hbar^2 a_{ib}}{\mu} \frac{1}{1 - \frac{2\pi\hbar^2 a_{ib}}{\mu} \frac{1}{V} \sum_{\mathbf{k}}^{\Lambda} \frac{2\mu}{\hbar^2 k^2}}.$$
 (1.41)

This expression immediately shows why contact interactions are to be treated with care: the relationship between the a priori meaningless parameter g_{ib} in the Hamiltonian and the physically relevant scattering length a_{ib} depends on the scale at which one is probing the physics through the cutoff Λ . The problem is not unique to Bose gases but commonly appears in other ultracold atomic systems where contact interactions are used, for example in Fermi gases. For a more in depth discussion of the problem in scattering theory we refer the interested reader to [60].

In practice this means that to establish the connection between g_{ib} and a_{ib} through (1.41), one first has to determine the extent to which the problem depends on the cutoff. A theory that is completely UV convergent in its momentum integrals is not probing the more intricate physics described in the corrections of the denominator in (1.41) and hence it is sufficient to use the lowest-order expression:

$$g_{ib}^{(0)} = \frac{2\pi\hbar^2 a_{ib}}{\mu}.$$
(1.42)

On the other hand, in the case that the momentum integrals diverge as a power of Λ such as observed in (1.38), this could indicate that the types of processes captured in the theory are probing the physics further that what is described by
$g_{ib}^{(0)}$ and a correction should be made up to lowest relevant order in Λ . This is obtained by expanding the denominator to obtain the lowest order dependence on a power of Λ :

$$g_{ib}^{(1)} = g_{ib}^{(0)} + \left(g_{ib}^{(0)}\right)^2 \frac{1}{V} \sum_{\mathbf{k}}^{\Lambda} \frac{2\mu}{\hbar^2 k^2} = g_{ib}^{(0)} + \left(g_{ib}^{(0)}\right)^2 \frac{1}{\pi^2} \frac{\mu\Lambda}{\hbar^2}.$$
 (1.43)

In expression (1.40), this substitution should only be made in the first term given that the second term already exhibits a UV divergence even at lowest order $g_{ib}^{(0)}$. This has the exact result of regularizing the divergence as performed in (1.39).

We will encounter these types of UV divergences of the polynomial type numerous times in this thesis. The important message here is that they are an artifact of using a constant g_{ib} for idealized contact interactions, whereas more care reveals that potential corrections $g_{ib}(\Lambda)$ are necessary for consistency. These divergences are well understood and have been encountered in various ultracold atomic systems where contact interactions are used to capture the low-energy collisions that do not probe the shape of the interatomic potential.

1.5.3 LANDAU-PEKAR APPROACH

The Landau-Pekar approach is based on the early theories of the solid state polaron of S.I. Pekar [2] following upon Landau's initial treatment of the problem [1]. The approach proposes a variational product ansatz to the problem without any entanglement between the impurity and phonons:

$$|\Psi\rangle = |\varphi\rangle_I \times |\alpha\rangle. \tag{1.44}$$

For the phonon state, once again a simple coherent state ansatz is used:

$$|\alpha\rangle = e^{\sum_{\mathbf{k}} f_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} - f_{\mathbf{k}}^* \hat{\alpha}_{\mathbf{k}}^\dagger} |0\rangle, \qquad (1.45)$$

and the impurity is assumed to be in a Gaussian state with some variational parameter for its width λ :

$$\varphi_I(\mathbf{r}) = A \exp\left(-r^2/\lambda^2\right).$$
 (1.46)

The main difference between this treatment and the more sophisticated Lee Low Pines approach is that the ansatz (1.44) is proposed in the lab frame without first performing the Lee Low Pines transformation. CHAPTER 1 - POLARONS

Regardless of its simplicity, this product ansatz in the lab frame turns out to be the exact ground state solution of the original LO Fröhlich model in the strong coupling limit $\alpha \to \infty$ [6]. Therefore, in the original Fröhlich model, the weak to intermediate coupling regime is captured by the Lee Low Pines treatment, whereas the strong coupling approach reduces to the Landau-Pekar ansatz. An all coupling approach that was capable of capturing both regimes has been first proposed by Feynman in 1955 [8] and will be discussed in the next subsection.

For the Bose polaron, the Landau-Pekar approach has one significant concern: the energy arising from ansatz (1.44) is UV convergent, while we have already seen that the Lee-Low-Pines approach that a Lippmann-Schwinger regularization procedure is necessary. The reason for this is the Gaussian ansatz (1.46) which sharply cuts off the high momentum behavior of the impurity and hence the UV behavior is not sufficiently probed. The simple Landau-Pekar approach can therefore not be quantitatively compared to other approaches where such regularization is necessary. This could perhaps be fixed by introducing a better guess for the impurity function $|\varphi\rangle_I$. However, as we will see, for the Bose polaron the adiabatic ansatz cannot capture the strong coupling regime anyway, in contrast to the original Fröhlich case. For this reason we will not be discussing the Landau-Pekar ansatz when comparing different approaches in the literature further on.

1.5.4 Feynman's variational path integral treatment

The superior method that interpolates the Lee Low Pines and Landau Pekar treatments for the original Fröhlich model has been proposed by Feynman in 1955 [8] based on his theory of path integrals. In this approach the Fröhlich Hamiltonian is transformed into an action functional form that can be used in the path integral formalism. We discuss the approach already immediately applied to the Bogoliubov-Fröhlich Hamiltonian (1.21), but the general case for any Fröhlich Hamiltonian can be trivially obtained by redefining the interaction strength used in this section to a more general one $(g_{ib}\sqrt{N_0}/V) V_k \rightarrow V_k$. The action functional equivalent to the Hamiltonian (1.21) for the path integral formalism in imaginary time [61] is given by:

$$\mathcal{S}_{\text{tot}}[\mathbf{r}, Q_{\mathbf{k}}] = \int_{0}^{\hbar\beta} \left(\frac{m\dot{\mathbf{r}}^{2}}{2} + \frac{M}{2} \sum_{\mathbf{k}} \dot{Q}_{\mathbf{k}}^{*} \dot{Q}_{\mathbf{k}} + \sum_{\mathbf{k}} \frac{M\omega_{\mathbf{k}}^{2}}{2} Q_{\mathbf{k}}^{*} Q_{\mathbf{k}} + \frac{\sqrt{N_{0}}g_{ib}}{V} \sum_{\mathbf{k}} \rho_{\mathbf{k}} \sqrt{\frac{2M\omega_{\mathbf{k}}}{\hbar}} V_{\mathbf{k}} Q_{\mathbf{k}} \right) d\tau.$$

$$(1.47)$$

In this formalism, the impurity operator has been promoted to a vector \mathbf{r} with a corresponding density $\rho_{\mathbf{k}} = \exp(i\mathbf{k}\cdot\mathbf{r})$, and the phonons are represented by an infinite set of scalar functions $\{Q_k\}$ with some mass M. Losing the quantum mechanical operator nature comes at a cost, the action functional does not depend on simply scalar values but on entire paths $\mathbf{r}(\tau)$ and $Q_{\mathbf{k}}(\tau)$ of the particles on the interval $[0, \hbar\beta]$. In the integral boundary, the inverse temperature $\beta = (k_B T)^{-1}$ appears, and hence thermal fluctuations can be naturally taken into account in this method. In general we will mostly be interested in the zero temperature limit $\beta \to \infty$. The difficulty of studying the ground state properties of the Fröhlich Hamiltonian (1.21), or the Hamiltonian formalism in general, is trying to understand the interplay between the Hamiltonian operator and the sets of states in the Hilbert space. For the path integral formalism, the difficulty of the problem is now transformed to something entirely different. To access the partition function of the system \mathcal{Z} , which contains the energy and other thermodynamic quantities, one has to be able to count over all possible paths $\mathbf{r}(\tau)$ and $Q_{\mathbf{k}}(\tau)$ exponentially suppressing their contribution by the value of the corresponding action functional (1.47). Formally this is written down as the many-body path integral:

$$\mathcal{Z} = \int \mathcal{D}\mathbf{r} \int \mathcal{D}Q_{\mathbf{k}} e^{-\mathcal{S}_{\text{tot}}[\mathbf{r}, Q_{\mathbf{k}}]/\hbar}, \qquad (1.48)$$

where the calligraphic differential \mathcal{D} symbolically indicates a sum over all paths of the corresponding variable. Technically, for the partition function only the cyclic paths have to be counted, but it is common to omit this condition in the notation since it is usually clear from the context. The path integral formalism allows one to do the opposite of the Lee Low Pines transformation. Instead of integrating out the impurity, now the phonons can be integrated out exactly:

$$\int \mathcal{D}Q_{\mathbf{k}} e^{-\mathcal{S}_{\text{tot}}[\mathbf{r}, Q_{\mathbf{k}}]/\hbar} = e^{-\mathcal{S}_{\text{eff}}[\mathbf{r}]/\hbar}.$$
(1.49)

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This completely eliminates the phonons from the problem and we can describe the single impurity by its *effective action* functional:

$$\mathcal{S}_{\text{eff}} = \int_0^{\hbar\beta} \frac{m\dot{\mathbf{r}}^2}{2} dt - \frac{1}{V} \sum_{\mathbf{k}} \frac{g_{ib}^2 n_0}{2\hbar} V_{\mathbf{k}}^2 \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma \mathcal{G}_{\mathbf{k}} \left(\tau - \sigma\right) \rho_{\mathbf{k}}(\tau) \rho_{\mathbf{k}}^*(\sigma), \quad (1.50)$$

where similar to the Lee Low Pines transformation, the impurity now experiences a difficult retarded interaction mediated by the Green's function of the excitations:

$$\mathcal{G}_{\mathbf{k}}(u) = \frac{\cosh\left[\omega_{\mathbf{k}}\left(|u| - \hbar\beta/2\right)\right]}{\sinh\left(\omega_{\mathbf{k}}\hbar\beta/2\right)}.$$
(1.51)

The remaining problem of computing the impurity path integral:

$$\mathcal{Z} = \int \mathcal{D}\mathbf{r} e^{-\mathcal{S}_{\text{eff}}[\mathbf{r}]/\hbar},\tag{1.52}$$

can not be solved analytically due to the non-quadratic interactions in the action functional (1.50).

To proceed semi-analytically, an approximation has to be made at this point. In his seminal paper on the polaron problem [8], Feynman just like his predecessors chooses for a variational approach. In the path integral approach a powerful variational inequality for the free energy is the Jensen-Feynman inequality [62]. This variational principle allows one to get an upper bound on the free energy of the real action functional of a system S based on a simpler variational model system with an action functional S_0 :

$$F \le F_0 + \frac{1}{\hbar\beta} \left\langle S - S_0 \right\rangle_0. \tag{1.53}$$

Here, the free energy F_0 corresponds to that of the model system and the expectation value $\langle ... \rangle_0$ is defined with respect to the trial action:

$$\left\langle A[\mathbf{r}(\tau)]\right\rangle_{0} = \frac{\int \mathcal{D}\mathbf{r}A[\mathbf{r}(\tau)]e^{-\mathcal{S}_{0}/\hbar}}{\int \mathcal{D}\mathbf{r}e^{-\mathcal{S}_{0}/\hbar}}.$$
(1.54)

Feynman's next idea was to propose a simpler model action S_0 to simulate the physics of the difficult effective action (1.50), but one that still can be dealt with analytically. The model system most often considered in this approach is shown in Figure 1.4 where the effect of the infinite set of phonons with a difficult coupling to the impurity is replaced by a simple fictitious particle with mass M and a harmonic coupling MW^2 . Similarly to what has been done for the effective action,



FIGURE 1.4: The model system initially proposed by Feynman in his seminal paper on the polaron [8], where a fictitious mass is harmonically coupled to the impurity.

the fictitious mass is integrated out to obtain the model action for the system at the same level as S_{eff} :

$$\mathcal{S}_{0} = \int_{0}^{\hbar\beta} \frac{m\dot{\mathbf{r}}^{2}}{2} dt + \frac{MW^{3}}{8} \int_{0}^{\hbar\beta} d\tau \int_{0}^{\hbar\beta} d\sigma \frac{\cosh\left[W\left(u - \hbar\beta/2\right)\right]}{\sinh\left(W\hbar\beta/2\right)} \left[\mathbf{r}(\tau) - \mathbf{r}(\sigma)\right]^{2}.$$
(1.55)

The action functional S_0 is still non-local in time, but the interaction term is quadratic in the impurity variables which allows to compute the path integrals of this system analytically. The variational free energy on the right hand side of the inequality (1.53) can now be analytically computed to be:

$$F_{v}(M,W) = \frac{3}{\beta} \log \left[\sinh\left(\frac{\hbar\beta\Omega}{2}\right) \right] - \frac{3}{\beta} \log \left[\sinh\left(\frac{\hbar\betaW}{2}\right) \right] - \frac{3}{2\beta} \log\left(\frac{m+M}{m}\right) - \frac{3}{2\beta} \frac{M}{M+m} \left[\frac{\hbar\beta\Omega}{2} \coth\left(\frac{\hbar\beta\Omega}{2}\right) - 1 \right] - \frac{g_{ib}^{2}n_{0}}{\hbar V} \sum_{\mathbf{k}} V_{\mathbf{k}}^{2} \int_{0}^{\hbar\beta/2} \mathcal{G}_{\mathbf{k}}(u) \mathcal{F}_{\mathbf{k}}(u) du, \quad (1.56)$$

where $\Omega = W\sqrt{1 + M/m}$ and:

$$\mathcal{F}_{\mathbf{k}}(u) = \exp\left(\frac{\hbar k^2}{2\left(M+m_I\right)} \left[\frac{u^2}{\hbar\beta} - u + \frac{M}{\Omega} \frac{\cosh\left(\Omega\left[\hbar\beta/2 - u\right]\right) - \cosh\left(\hbar\beta\Omega/2\right)}{\sinh\left(\hbar\beta\Omega/2\right)}\right]\right).$$
(1.57)

This calculation has been first performed for the Bose polaron in [48] where the interested reader can find the technical details of the calculation. In Chapter 2 we will also present a far more general calculation from which this expression could be found as well. The variational free energy (1.56) also contains the same $\sim \Lambda$ UV divergence that can be removed through Lippmann-Schwinger regularization.

The hope is to find a close approximation the free energy of the real system

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by minimizing F_v with respect to the variational parameters M and W, which is guaranteed to yield an upper bound by the Jensen inequality. Strictly speaking, it cannot be excluded that while S_0 produces a good upper bound to the energy it could completely miss other polaronic quantities such as the effective mass. This problem has however not been encountered before and it turns out that S_0 produces a good description of the other polaronic quantities as well [63].

1.5.5 CORRELATED GAUSSIAN WAVEFUNCTIONS

In the context of the Bogoliubov-Fröhlich model, the method of correlated Gaussian wavefunctions has been applied to the problem in [64]. This method is based on variational coherent squeezed states more commonly encountered in photonics, which have been previously proposed for polaron theory in [65–67]. Here, we briefly summarize the method. The general idea is to start in the impurity frame after the Lee Low Pines transformation, but now improve on the coherent state ansatz for the phonon function proposed in (1.35). The crucial step lies in adding an additional squeezing transformation which introduces entanglement between phonon modes at different momenta \mathbf{k} and \mathbf{k}' :

$$|CGW\rangle = e^{\sum_{\mathbf{k}} f_{\mathbf{k}} \hat{\alpha}^{\dagger}_{\mathbf{k}} - hc} \left(e^{\sum_{\mathbf{k},\mathbf{k}'} Q_{\mathbf{k},\mathbf{k}'} \hat{\alpha}^{\dagger}_{\mathbf{k}} \hat{\alpha}^{\dagger}_{\mathbf{k}'} - hc} \right) |0\rangle, \qquad (1.58)$$

where the variational parameters of the state are the functions $f_{\mathbf{k}}$ and $Q_{\mathbf{k},\mathbf{k}'}$. The presence of the squeezing transformation significantly complicates the minimization procedure and the optimal $Q_{\mathbf{k},\mathbf{k}'}$ has to be found numerically. In the initial discussions of this method in the context of the original Fröhlich model this minimization was deemed too difficult and approximate solutions were given [66, 67]. However, the more recent paper where this method is applied to the Bogoliubov-Fröhlich model [64] presents a new way of performing the minimization. This allows the authors to variationally minimize the energy of the coherent squeezed state $E[f_{\mathbf{k}}, Q_{\mathbf{k},\mathbf{k}'}]$ for the Bose polaron. Very recent extensions of this method to the attractive polaron branch in the extended Fröhlich model can be found in [45].

1.5.6 RENORMALIZATION GROUP THEORY

Renormalization group (RG) theory is a mathematical formalism, most commonly used in statistical and quantum field theories, that studies the symmetries of a class of transformations associated with the momentum cutoff Λ of the system. RG theory applications to both the Bogoliubov-Fröhlich Hamiltonian and its extended versions [68–70] will form important references in the discussion of the next chapters. For this reason we present a very brief discussion of renormalization group (RG) theory for the interested reader based on the introduction in Shankar's review on this topic [71]. Since RG theory is quite technical and we will not be needing the details in this thesis, we mainly focus on a conceptual discussion.

As the name suggests, RG has its roots in the procedure of renormalization of quantum field theories. Imagine a quantum field theory with one or multiple coupling constants α (such as the mass, interaction strength, etc.) where a finite cutoff Λ is placed on all momentum integrals associated with the underlying field $\phi(\mathbf{k})$. In contrast to problems in condensed matter physics, where a natural cutoff value for Λ exists, one is eventually interested in understanding the theory at $\Lambda \to \infty$. However, in this limit often divergences can arise in the quantities of interest such as the energy. The way that this problem can sometimes be dealt with is to allow for the possibility that the coupling constants themselves depend on the cutoff $\alpha \to \alpha$ (Λ) in such a way that the quantities of interest come out to be finite.

It turns out that this point of view can be incredibly useful to study systems even where the momentum cutoff is finite. In particular, renormalization group theory presents a systematic way to understand the difference between physics at small and large momenta of a system, a question that can also be of interest even if some large momentum cutoff Λ will not be sent to infinity. The general concept of RG can be simply summarized as follows. Let us define an action functional $S_{\Lambda}[\phi]$ of a quantum field at some momentum cutoff Λ , where all field contributions in momentum space below some $\Lambda' < \Lambda$ are called ϕ_1 and all contributions in the shell $\Lambda' are called <math>\phi_2$. Here, one can imagine the phonons of, for example, the Bogoliubov-Fröhlich model to correspond to the momentum modes of such a field. It is at least then in principle possible to integrate out the fast contributions:

$$\int \mathcal{D}\phi_2 e^{-S_\Lambda[\phi]} = e^{-S'[\phi_1]} \tag{1.59}$$

to obtain an effective action of the slow field $S'[\phi_1]$. After a number of additional transformations where the new momentum domain and the remaining field ϕ_1 get rescaled, RG theory attempts to map the new effective action $S'[\phi_1]$ onto the old functional $S_{\Lambda}[\phi]$ with modified coupling constants α' . Of course, this is merely the general concept and in practice way more technical details are involved but fall Chapter 1 - Polarons

beyond the scope of this discussion.

Renormalization Group theory became well known in condensed matter physics in the context of the Kondo problem [72] which is the problem of understanding the properties of conducting electrons in the presence of magnetic impurities in the material which can induce a spin flip on a conducting electron. In particular, any type of perturbative calculation failed at zero temperature as the resistivity appeared to have an unphysical logarithmic divergence $\sim \ln(T)$. The first successful approach to the problem was through renormalization group theory by Anderson [73], where the solution consisted out of approximately integrating out the energy scales as outlined in the previous paragraph. This problem has been later more rigorously solved by Wilson [74] establishing the foothold of RG approaches to condensed matter physics.

Renormalization Group theory approaches conceptually similar to Anderson's *poor man's scaling* theory [73] have been successfully employed in a series of papers to analyze the ground state properties of the Bogolibuov-Fröhlich [68, 69] model and the extended Bogolibov-Fröhlich model [70]. In the next chapter we will start by discussing and comparing the various theoretical approaches outlined in this chapter to the Bogolibov-Fröhlich model.

CHAPTER 2

The path integral approach for the Bogoliubov-Fröhlich model

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In this chapter we start by comparing the different theoretical approaches that have been introduced in the previous section for the Bogoliubov-Fröhlich model. As has been observed in the literature and will be discussed here, Feynman's variational path integral approach exhibits discrepancies with diagrammatic Monte Carlo (diagMC) calculations when the cutoff Λ in the model is large. The goal of this chapter is to discuss the issues of Feynman's approach and show how the approach can be improved. This result lays the foundation for exploring the path integral approach further in the rest of the thesis.

2.1 Feynman's all coupling approach

We start the chapter by briefly reviewing Feynman's variational path integral approach [8] that was introduced in Chapter 1 and has since its inception been regarded as the semi-analytical tool of choice to study the Fröhlich Hamiltonian [4]. For any general Fröhlich Hamiltonian of the form (1.29) with an interaction amplitude $\tilde{V}_{\mathbf{k}}$, the phonon degrees of freedom can be integrated out exactly at the Chapter 2 - The path integral approach for the Bogoliubov-Fröhlich model

level of the partition function:

$$\mathcal{Z} = \int \mathcal{D}\mathbf{r} \ e^{-\mathcal{S}_{\text{eff}}[\mathbf{r}]/\hbar}.$$
 (2.1)

This can be shown to yield an *effective action* S_{eff} where the impurity is interacting with itself at previous times:

$$\mathcal{S}_{\text{eff}} = \int_{0}^{\hbar\beta} \frac{m\dot{\mathbf{r}}^{2}}{2} d\tau - \sum_{\mathbf{k}} \frac{1}{2\hbar} \left| \tilde{V}_{\mathbf{k}} \right|^{2} \int_{0}^{\hbar\beta} d\tau \int_{0}^{\hbar\beta} d\sigma \ \mathcal{G}_{\mathbf{k}} \left(\tau - \sigma \right) e^{i\mathbf{k} \cdot \left[\mathbf{r}(\tau) - \mathbf{r}(\sigma) \right]}$$
(2.2)

where:

$$\mathcal{G}_{\mathbf{k}}(u) = \frac{\cosh\left[\omega_{\mathbf{k}}\left(|u| - \hbar\beta/2\right)\right]}{\sinh\left(\omega_{\mathbf{k}}\hbar\beta/2\right)}.$$
(2.3)

A variational upper bound for the free energy corresponding to the effective action can be found in terms of a simpler *model action* S_0 :

$$F \le F_0 + \frac{1}{\hbar\beta} \left\langle \mathcal{S}_{\text{eff}} - \mathcal{S}_0 \right\rangle.$$
(2.4)

Feynman's original proposal for the model action [8, 62], given in expression (1.55) of Chapter 1, consists out of a coupled harmonic oscillator with two variational parameters, where one of the particles has been integrated out to simulate the memory effects. The method to obtain the upper bound to the free energy therefore comes down to minimizing the right hand side of (2.4) as a function of two variational parameters which can numerically be easily performed.

Regardless of its simplicity, in previous studies of the Fröhlich model Feynman's approach shows remarkable agreement with diagrammatic Monte Carlo (diagMC) calculations for the optical polaron [75] and the acoustic polaron [10] as illustrated in Figure 2.1. Diagrammatic Monte Carlo is a computationally demanding approach in which the sum over all non-negligible Feynman diagrams of the problem is performed until the ground state energy is converged. Therefore, at least in principle, Monte Carlo methods provide *exact* solutions for the Hamiltonian under investigation and provide an excellent gauge for comparison to other theoretical methods. Having such a powerful, but in some aspects opaque, computational method is a significant advance. Nevertheless, it does not imply the end of theoretical investigation and there are various reasons to try and understand the physics of the problem from different angles. Even in light of ever increasing processing power, Monte Carlo methods still remain computationally demanding to this day and require access to supercomputers with hundreds of nodes. In addition, as we will also encounter further in this chapter, knowing how to capture the physical state and the processes that are most relevant for a particular physical quantity in a simpler theory often provides a deeper understanding of the system.



FIGURE 2.1: A comparison between the polaronic ground state energy in Feynman's approach and diagrammatic Monte Carlo performed by Vlietinck et al. [10] for the optical polaron (left panel) and for the acoustic polaron (right panel). Figure adapted from [10].

Returning to Feynman's path integral method, at weak and strong coupling the approach reduces to respectively the coherent state Lee-Low-Pines method [7] and the strong-coupling Landau-Pekar ansatz¹ [2] and has for this reason also been called *the all-coupling approach* for the optical Fröhlich model. Two distinct ways to improve even further upon Feynman's original proposal can be found in the literature. First, the model action can be generalized to the best quadratic action functional [76, 77], which yields an improvement to Feynman's result for the ground state energy below 0.15%. Second, corrections beyond the first order variational expansion can be made [78, 79] and yield improvements upon Feynman's result below 1.6%. These results provide an additional confirmation of the astounding accuracy of the simple coupled oscillator model in solid state polaron theory. It should be emphasized that, while this is true for the ground state energy, for the dynamical response of the system, an application of the best quadratic action to the optical polaron yields much larger improvements [80].

In this chapter we will focus on the application of Feynman's approach to the

¹Note that this is true for the optical or acoustic Fröhlich model, but in the Bogoliubov-Fröhlich model Pekar's ansatz does not capture the Lippmann-Schwinger regularization.

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Bogoliubov-Fröhlich Hamiltonian that has been introduced in Chapter 1:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}^{\dagger}_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} + \frac{\sqrt{N_0} g_{ib}}{V} \sum_{\mathbf{k}} V_{\mathbf{k}} e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} \left(\hat{\alpha}^{\dagger}_{-\mathbf{k}} + \hat{\alpha}_{\mathbf{k}} \right), \qquad (2.5)$$

where:

$$\hbar\omega_{\mathbf{k}} = \sqrt{\frac{\hbar^2 k^2}{2m_b} \left(\frac{\hbar^2 k^2}{2m_b} + 2g_{bb}n_0\right)},$$
(2.6)

$$V_{\mathbf{k}} = \left(\frac{\frac{\hbar^2 k^2}{2m_b}}{\frac{\hbar^2 k^2}{2m_b} + 2g_{bb}n_0}\right)^{1/4}.$$
(2.7)

Whereas in the original Fröhlich Hamiltonian, $\omega_{\mathbf{k}}$ is the constant frequency of longitudinal optical phonons and $V_{\mathbf{k}}$ tends to zero at large momenta, in the Bogoliubov-Fröhlich Hamiltonian the coupling amplitude remains finite and the excitation spectrum becomes particle-like. This seemingly innocuous change has dramatic consequences for the UV behavior of the model, which from a mathematical physics point of view does not fall into any class of UV divergencies previously encountered in Fröhlich-like Hamiltonians [56].

It is important to emphasize that beyond weak coupling between the impurity and the gas, the physics of the Bose polaron is not accurately captured by the Bogoliubov-Fröhlich Hamiltonian (2.5). At stronger interactions the Bogoliubov approximation appears to suffer from an instability for attractive polarons [70, 81] which was explored in great detail in a more recent study [82]. In addition, inclusion of higher order interactions on top of the lowest-order Fröhlich coupling term have been considered and were shown to be of importance [49, 50, 70, 81]. Finally, Efimov physics has also been shown to play an important role in the ground state of the attractive Bose polaron [42–45] which are not captured within the non-extended Fröhlich model. In the rest of this chapter, we will solely focus on a discussion of the Bogoliubov-Fröhlich model (2.5) with repulsive effective interactions g_{ib} . The discussion will also concern results at stronger coupling, which are not to be interpreted as a prediction for the Bose polaron in that regime, but rather as a testing ground for corrections to the path-integral approach.

2.2 New theoretical approaches

The Bogoliubov-Fröhlich model has been studied within this approach [48], where Feynman's original S_0 has been used [62]. Just as is the case for the solid state polaron, the variational upper bound reduces to the coherent state energy at weak coupling [58] and is capable of providing an adiabatic ansatz at strong coupling and hence was expected to work well for this Hamiltonian. However, not long afterwards, very unexpectedly large discrepancies between the theory and rigorous diagMC calculations [10] have been observed. In addition to the previously discussed well known linear UV divergence in the momentum integrals, associated with using contact interactions, a novel logarithmic UV divergence was argued to be present in the diagMC study [68]. The logarithmic UV behavior is completely absent in the variational approach [48], which is indicative of new physics that is not captured within the approach.

In an impressive series of papers by *F. Grusdt et al.*, employing a renormalization group (RG) theory [57, 68, 69, 83], and by *Shchadilova et al.* employing correlated Gaussian wavefunctions (CGW) [64], the Bogoliubov-Fröhlich model has been studied in great detail. The authors show that the ground state of the Bogoliubov-Fröhlich Hamiltonian contains entangled phonon modes at different energies [64], and that adequately capturing quantum fluctuations in the RG or CGW approaches gives rise to the logarithmic UV divergence in the momentum cutoff of the ground state energy that has been observed in diagMC calculations [10]. The momentum cutoff Λ therefore plays an important role in the problem, dictating the importance of quantum fluctuations. In particular, at large cutoff in the intermediate coupling regime $\alpha \approx 1$, the phonons are argued to be strongly correlated forming the most challenging theoretical regime.

The comparison between the different methods in the literature is presented in Figure 2.2 for the system parameters of a light ⁶Li impurity immersed in a heavier ²³Na condensate with $m_b = 3.8m$ that have been used in the diagMC study [10]. As shown in [69], it turns out that the subtleties discussed in this chapter are more prominent for a lighter impurity mass and hence this choice is excellent for the purpose of comparison between different approaches. When compared at small cutoff values and strong coupling, the Jensen-Feynman approach performs better than perturbative RG [68] or CGW [64], and is in good agreement with diagMC [10]. However, when Λ is large, Feynman's approach fails to completely capture the quantum fluctuations and the other approaches provide a far more accurate

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FIGURE 2.2: The comparison between various existing theoretical approaches for the Bogoliubov-Fröhlich Hamiltonian. The polaronic contribution of the ground state energy is presented as a function of the (repulsive) polaronic coupling constant α for (a)-(c), and as a function of the momentum cutoff Λ but at fixed $\alpha = 3$ in (d). The Monte Carlo results from [10] are presented as red squares (with error flags), the black dotted line is the Lee Low Pines approach [7], the dashed green line is Feynman's approach [48], the red dashdotted line is perturbative RG [68] and the red solid line is CGW [64]. Results are presented at zero temperature for a mass ratio $m_b = 3.8m$.

description, in particular at weak and intermediate coupling. More recently, the perturbative RG approach has been extended to also work well at strong coupling [83] lifting it to the status of an all-coupling approach. On the other hand, CGW [64] works well at weak to intermediate coupling but shows significant discrepancies with diagMC towards strong coupling. It is curious to note that in the study of the original Fröhlich model, Feynman's approach is celebrated precisely for its ability to capture quantum fluctuations when compared to adiabatic density functional theory [84], which only emphasizes the elusiveness of the Bogoliubov-Fröhlich model in comparison to its solid state counterpart.

Although the Bogoliubov-Fröhlich Hamiltonian is now better understood, nevertheless the question remains as to why Feynman's approach fails or how it can be improved. This can be of interest purely from a mathematical point of view [56], or as a first step towards future applications to multiple particles in this model or extended Fröhlich Hamiltonians [50]. Most important of all, the aim of starting with this chapter is to show the reader, who might have heard of the issues surrounding Feynman's approach in the context of the Bose polaron discussed in the previous paragraphs, that the path integral method can be significantly improved. The central technical goal of this chapter is therefore to use the Bogoliubov-Fröhlich model as an illustration of the importance of further corrections to the path integral method when applied to polaronic models where quantum fluctuations cause additional UV divergences.

Note that in [68], a regularization procedure of this UV divergence is proposed through effective mass corrections to the mean field impurity-condensate interactions term $g_{ib}n_0$, which we have not included in the Hamiltonian (2.5). Here, we will not be concerned with this regularization since the goal is specifically to discuss the mechanism of appearance of this UV behavior in Feynman's approach. Moreover, for an accurate comparison with realistic experiments the cutoff Λ should be related to either the inverse van der Waals length of the atomic potential [48, 70] or the first Efimov resonance [45]. For the current system the former value corresponds to $\Lambda \approx 200\xi^{-1}$, and in what follows figures will be presented with results up to $\Lambda \approx 4000\xi^{-1}$. For this reason, in addition to the Bogoliubov-Fröhlich model being only valid at weak coupling, we emphasize that the results in their current form are not suitable for direct comparison with experiment.

In this chapter we show that two modifications bring significant improvements to Feynman's approach for the Bogoliubov-Fröhlich Hamiltonian. In Sec. 2.3 we consider the best quadratic action functional [77] as the model action for this

system. While this correction is extremely small in the Fröhlich model, we show that the largest correction to the ground state energy of the Bogoliubov-Fröhlich model is obtained in this step. We obtain the optimal memory kernel which also provides insights as to why Feynman's original model fails. At strong coupling the results show good agreement with diagMC, but near the challenging intermediate coupling regime some noticeable discrepancy remains.

To obtain further corrections for the intermediate regime, in Sec. 2.5 we derive an expression for the correction from the second-order cumulant expansion of the partition function. This correction has been shown to be small [78, 79] in the Fröhlich model, but turns out to be appreciable for the Bogoliubov-Fröhlich model. Combining the two aforementioned improvements, we retrieve the logarithmic divergence of the model and find excellent agreement with diagMC in the intermediate regime.

2.3 Quadratic action with a general memory kernel

The derivation presented here has been performed for the optical Fröhlich model in [76], and further addressed in [77]. Contrary to the treatment in [76, 77], the Bogoliubov-Fröhlich model (2.5) is more difficult in the sense that the momentum integrals cannot be analytically performed. The results obtained here can therefore be applied to any general Fröhlich Hamiltonian. The central quantity in this section will be the model action functional (working in units of $\hbar = 1$ from now on):

$$S_0 = \frac{m}{2} \int_0^\beta \dot{\mathbf{r}}^2 d\tau + \frac{m}{2\beta} \int_0^\beta \int_0^\beta d\tau d\sigma \ x(\tau - \sigma) \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma).$$
(2.8)

The crucial step here is that we propose a general memory kernel $x(\tau - \sigma)$ with far greater freedom than the commonly used Feynman model action. Note that introducing an additional β in the denominator of the second term in (2.8) is purely for convenience of notation further on. Following [76], we make the restriction to β -periodic functions $x(\beta - \tau) = x(\tau)$ and in addition assume $\int_0^\beta x(\tau)d\tau = 0$. While the first assumption is necessary for the derivation, the second could in principle be relaxed [76]. The variational free energy (2.4) instead of being a function of two variational parameters M and W, as would be the case in Feynman's original 2.3 - Quadratic action with a general memory kernel

model, is now a functional of the memory kernel $x(\tau - \sigma)$:

$$F_{v}[x] = F_{0} + \frac{1}{\beta} \left\langle \mathcal{S}_{\text{eff}} - \mathcal{S}_{0} \right\rangle.$$
(2.9)

Since the action functional is quadratic in the impurity degree of freedom, exact expressions for all quantities in (2.9) can be obtained. In what follows we largely follow the steps of [76], now applied to the Bogoliubov-Fröhlich model.

In principle, all expectation values of analytic functions of $\mathbf{r}(\tau)$ can be computed via a generating function, which satisfies the following identity for any vector function $\mathbf{g}(\tau)$ (in three dimensions):

$$\left\langle \exp\left(\int_{0}^{\beta} \mathbf{g}(\tau) \cdot \mathbf{r}(\tau) d\tau\right) \right\rangle = \exp\left(\frac{1}{6} \int_{0}^{\beta} \int_{0}^{\beta} \langle \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma) \rangle \, \mathbf{g}(\tau) \cdot \mathbf{g}(\sigma) d\tau d\sigma\right). \tag{2.10}$$

The property of β -periodicity allows to decompose the memory kernel in Fourier space:

$$x(u) = \sum_{n = -\infty}^{\infty} x_n e^{i\nu_n u}$$
(2.11)

with Matsubara frequencies $\nu_n = 2\pi n/\beta$. The covariance in expression (2.10) is nothing else than the Green's function of the corresponding classical equation of motion, as commonly encountered in introductory quantum field theory [85]. Here, it can also be obtained in first quantization:

$$\langle \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma) \rangle = \frac{6}{m\beta} \sum_{n=1}^{\infty} \frac{\cos\left[\nu_n(\tau-\sigma)\right]}{\nu_n^2 + x_n}.$$
 (2.12)

Expressions (2.10) and (2.12) are not new and have been derived in previous works on this topic [76]. For the interested reader we note that this result can be easily obtained using the propagator (4.7) from Chapter 4 for any vector function where $\int_0^\beta \mathbf{g}(\tau) d\tau \neq 0$, which all the functions $\mathbf{g}(\tau)$ used in this chapter obey.

If an auxiliary parameter λ is introduced in the action functional (2.8) as a scaling factor to the memory kernel $x(\tau - \sigma) \rightarrow \lambda x(\tau - \sigma)$, the partition function \mathcal{Z} and free energy F_0 obtain a λ dependence:

$$\mathcal{Z}^{(\lambda)} = e^{-\beta F_0^{(\lambda)}} = \int \mathcal{D}\mathbf{r} e^{-\frac{m}{2}\int_0^\beta \dot{\mathbf{r}}^2 d\tau + \frac{m}{2\beta}\int_0^\beta \int_0^\beta d\tau d\sigma \ \lambda x(\tau - \sigma)\mathbf{r}(\tau) \cdot \mathbf{r}(\sigma)}$$
(2.13)

By defining the expectation value with respect to the scaled action functional in

(2.13) as $\langle\rangle_\lambda$ it can be readily shown that:

$$\frac{\partial F_0^{(\lambda)}}{\partial \lambda} = \frac{m}{2\beta^2} \int_0^\beta \int_0^\beta x(\tau - \sigma) \left\langle \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma) \right\rangle_\lambda d\tau d\sigma.$$
(2.14)

For the covariance this essentially corresponds to changing x_n to λx_n in (2.12). Expression (2.14) can now be integrated over λ to obtain the free energy of the model system:

$$F_0^{(\lambda)} = -\frac{1}{\beta} \log\left[\left(\frac{m}{2\pi\beta}\right)^{3/2} V\right] + \frac{3}{\beta} \sum_{n=1}^{\infty} \log\left(1 + \frac{\lambda x_n}{\nu_n^2}\right).$$
(2.15)

The kinetic energy contributions to the action functionals cancel in the second term of (2.9) and hence it is useful to redefine \tilde{S}_0 and \tilde{S}_{eff} , where the absence of the kinetic energy terms is emphasized by the tilde:

$$\tilde{\mathcal{S}}_{0} = \frac{m}{2\beta} \int_{0}^{\beta} \int_{0}^{\beta} d\tau d\sigma \,\,\lambda x(\tau - \sigma) \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma), \qquad (2.16)$$

$$\tilde{\mathcal{S}}_{\text{eff}} = -\frac{1}{V} \sum_{\mathbf{k}} \frac{g_{ib}^2 n_0}{2\hbar} V_{\mathbf{k}}^2 \int_0^{n_0} d\tau \int_0^{n_0} d\sigma \ \mathcal{G}_{\mathbf{k}} \left(\tau - \sigma\right) e^{i\mathbf{k} \cdot [\mathbf{r}(\tau) - \mathbf{r}(\sigma)]}.$$
(2.17)

By once again introducing the auxiliary variable and taking the derivative of the partition function with respect to λ , one can show:

$$\frac{1}{\beta} \left\langle \tilde{\mathcal{S}}_0 \right\rangle = \left. \frac{\partial F_0^{(\lambda)}}{\partial \lambda} \right|_{\lambda=1} = \frac{3}{\beta} \sum_{n=1}^{\infty} \frac{x_n}{x_n + \nu_n^2}.$$
(2.18)

The generating function result (2.10) also immediately yields the expectation value of the effective action (2.2). Note that the covariance (2.12) only depends on the time difference $|\tau - \sigma|$ and is in addition β -periodic. In the limit of zero temperature $\beta \to \infty$ this simplifies the double time integral from (2.2) to:

$$\frac{1}{\beta} \left\langle \tilde{S}_{\text{eff}} \right\rangle = -\frac{g_{ib}^2 n_0}{V} \sum_{\mathbf{k}} V_{\mathbf{k}}^2 \int_{0}^{\beta/2} \mathcal{G}_{\mathbf{k}}(u) \mathcal{F}_{\mathbf{k}}(u) du \qquad (2.19)$$

where:

$$\mathcal{F}_{\mathbf{k}}(u) = \exp\left(-\frac{2k^2}{m\beta}\sum_{n=1}^{\infty}\frac{1-\cos(\nu_n u)}{x_n+\nu_n^2}\right).$$
(2.20)

In the $\beta \to \infty$ limit the Matsubara summations in the previous expressions be transformed into frequency integrals, where the coefficients x_n become the Fourier transform $x(\nu)$ of the memory kernel (notation not to be confused with the original function):

$$\mathcal{F}_{\mathbf{k}}(u) = \exp\left(-\frac{k^2}{\pi m}\int_0^\infty d\nu \frac{1-\cos(\nu u)}{x(\nu)+\nu^2}\right).$$
(2.21)

Expression (2.19) contains a linear divergence in the momentum summation and is regularized by relating g_{ib} to the s-wave scattering length a_{ib} up to second order in the Lippmann-Schwinger equation in the Bose-polaron mean-field energy $g_{ib}n_0$ [48] as has also been extensively discussed in Chapter 1. This regularization eventually comes down to simply using the lowest-order expression for $g_{ib} = 2\pi\hbar^2 a_{ib}/\mu$, where $\mu^{-1} = m^{-1} + m_b^{-1}$ is the reduced impurity-boson mass, but now subtracting the divergent behavior from (2.19). For the Bose intraspecies interaction a lowest order expression $g_{bb} = 4\pi\hbar^2 a_{bb}/m$ is sufficient. Note that this regularization procedure is not related to the phonon entanglement discussed in the introduction.



FIGURE 2.3: The ground state energy at zero temperature ($\beta = 200$ used as a cutoff) for (a) moderate $\Lambda = 100\xi^{-1}$ and (b) large $\Lambda = 3000\xi^{-1}$ cutoff values, compared to the results taken from diagrammatic Monte Carlo calculations [10] (scatter squares). The dashed line shows an application of Feynman's original model [48] to this system, while the solid line is our result obtained with the general quadratic memory kernel. Note that for this comparison the energy scale is defined using the boson mass $m_b = 3.8m$.

Unless specified otherwise, in the rest of the chapter we will use polaronic units in terms of the impurity mass m = 1, the condensate healing length $\xi =$ Chapter 2 - The path integral approach for the Bogoliubov-Fröhlich model

 $\hbar/\sqrt{2m_bg_{bb}n_0} = 1$, and the corresponding energy scale $\hbar^2/(m\xi^2) = 1$, which also corresponds to setting $\hbar = 1$. This rescaling has been performed in [48] and will appreciably simplify the obtained expressions. For any physical analysis one can unambiguously transform back into appropriate units. In the rest of this chapter the mass ratio $m_b = 3.8m$ is used for all the figures for comparison with the diagMC results of [10]. Note that to facilitate comparison with [10] where the boson mass m_b was preferred as the mass unit, an appropriate energy rescaling is performed on the figures. We can now introduce the dimensionless coupling constant of this model [48] as:

$$\alpha = \frac{a_{ib}^2}{a_{bb}\xi},\tag{2.22}$$

which makes the direct connection to polaronic physics in solids. Combining all of the previous terms, taking the $\beta \to \infty$ limit, and also taking the volume V to infinity, allows one to write the variational functional as:

$$F_{v}[x] = \frac{3}{2\pi} \int_{0}^{\infty} d\nu \left[\log\left(1 + \frac{x(\nu)}{\nu^{2}}\right) - \frac{x(\nu)}{x(\nu) + \nu^{2}} \right] - \frac{\alpha}{4\pi\mu^{2}} \int_{0}^{\Lambda} dk \ k^{2} V_{\mathbf{k}}^{2} \int_{0}^{\beta/2} \mathcal{G}_{\mathbf{k}}(u) \mathcal{F}_{\mathbf{k}}(u) du + \frac{\alpha\Lambda}{2\pi\mu}.$$
(2.23)

Here, Λ is the finite momentum cutoff discussed in Chapter 1, and the final term arises from the contact interaction regularization. The functional that minimizes the energy is found by taking the derivative with respect to a discrete Fourier component $\partial_{x_n} F_v = 0$ before the continuum limit is taken. Once the continuum limit is taken, the following integral equation can be obtained for the memory kernel:

$$x(\nu) = \frac{\alpha}{3\pi\mu^2} \int_0^{\Lambda} dk \ k^4 V_{\mathbf{k}}^2 \int_0^{\beta/2} \mathcal{G}_{\mathbf{k}}(u) \mathcal{F}_{\mathbf{k}}(u) \sin\left(\frac{\nu u}{2}\right)^2 du.$$
(2.24)

Since $\mathcal{F}_{\mathbf{k}}(u)$ is itself a functional of $x(\nu)$ this equation has to be solved numerically. This is done iteratively, starting by substituting the Lee-Low-Pines solution $x(\nu) = 0$ into the right-hand side of (2.24) and obtaining an improved memory kernel on the left-hand side. Depending on α , roughly one to ten iterations are needed until the relative increase in the corresponding energy (2.23) becomes less than 1%, which we accept as our final value. The next iteration yields further corrections of the order of 0.1% and can no longer be discerned on the graphs showed in this manuscript. We find that the frequency at which the memory kernel reaches an asymptotic value can become very large. For this reason we perform a scaling transformation $\nu = e^z - 1$ and select N = 1000 Gauss-Legendre quadrature points on the z-grid up to $\nu_{max} = 10^8$. The iterative improvement (2.24) is then performed for each point.

The results are shown in Figure 2.3 where we compare the ground state energy (2.23) for the optimized memory kernel with diagMC results from [10]. As already observed in [10, 64, 68], the original Feynman model yields surprisingly large discrepancies at strong coupling, especially at larger values of the cutoff $\Lambda = 3000\xi^{-1}$. This indicates that even in the limit of strong coupling quantum fluctuations are of importance and the adiabatic ansatz included in Feynman's model fails. We can see that the result for the best quadratic action functional (2.23) provides significant corrections to Feynman's model and yields a variational bound in good agreement with diagMC at strong coupling. However, as will be shown in Figure 2.7 in the next section, in the challenging intermediate coupling regime some discrepancies remain. To estimate corrections in this region, in the next section we consider further corrections beyond the first order variational inequality.

Let us also pay some attention to the optimized memory kernel itself. In Figure 2.4 we show the obtained optimized solutions for $x(\nu)$ that lead to the results shown in Figure 2.3. We can see that the UV limit of $x(\nu)$ agrees with the analytic expression $x(\nu) = \frac{\alpha}{6\pi\mu^2} (2\mu\Lambda^3/3)$. This limit can be readily obtained by substituting the mean field guess $x(\nu) = 0$ in the RHS of (2.24) and then taking the $\nu \to \infty$ limit. Therefore, it appears that in the Bogoliubov-Fröhlich model the UV limit of the optimal memory kernel does not converge as $\Lambda \to \infty$. On the other hand, we have checked that the small frequency behavior shown on the inset of Figure 2.4 is only very weakly influenced by the cutoff (while it does depend on α).

Finally, in Figure 2.5 we compare the shape of the optimized memory kernel to Feynman's original model, which is given by $x_{\text{Feyn}}(\nu) = MW^2\nu^2/(\nu^2 + W^2)$. The memory kernel tends to zero quadratically in ν , in the $\nu \to 0$ limit. This can be analytically shown in the first iteration by expanding expression (2.24) to lowest order in ν , and for the optimized solution this behavior is shown in the inset of Figure 2.4. However, as can be seen in the inset of Figure 2.5, the quadratic behavior rapidly transitions into an extended linear regime. In principle, the



FIGURE 2.4: The optimized memory kernel $x(\nu)$ at $\Lambda = 3000\xi^{-1}$ (in polaronic units) obtained for the energy plot in Figure 2.3b at three different coupling strengths $\alpha = 1, 2, 3$. The main plot shows the behavior at large ν on a logarithmic frequency axis, whereas the inset indicates a quadratic behavior at small frequencies. The dashed lines represent the analytic $\nu \to \infty$ limit mentioned in the text.

memory kernel of Feynman's model system exhibits a similar behavior, it starts of quadratic and then transitions into a linear regime before moving to an asymptotic value. The problem however is that Feynman's model has only two variational parameters so that the ranges of the regimes can not all be chosen independently. The quadratic behavior at small frequencies is dictated by the parameter MW^2 while the transition into the linear regime depends on W^2 in the denominator. This forces the memory kernel of Feynman's model system to make a compromise and reach its asymptotic value far more quickly than the general solution.

2.4 Effective mass

When an impurity is immersed in a medium, it should come as no surprise that its resistance to acceleration might become greater than the bare impurity mass. At small velocities the impurity can therefore be described as having an *effective* mass $m_{\text{eff}} > m$, a concept well known from the solid state polaron models [51, 52]. If the polaron system is to be modeled by Feynman's model action, the total mass in the model m + M provides a first rough approximation of the effective mass of

2.4 - Effective mass



FIGURE 2.5: A comparison between the general optimized memory kernel $x(\nu)$ and Feynman's original memory kernel. Inset shows the same plot at smaller frequencies. Plots are made at $\Lambda = 3000\xi^{-1}$ and $\alpha = 5$.

the polaron [62]. The study of the effective mass in the Bogoliubov-Fröhlich model at this level has been performed [48]. Although this simple approximation works incredibly well for the optical Fröhlich model [8, 62] the more general formula discussed in [8] and [86] should be used for other Fröhlich Hamiltonians to obtain a more accurate expression for the effective mass. The effective mass of the Bogoliubov-Fröhlich model has been compared between Feynman's approach and CGW or RG in [64, 68, 83]. In particular, the comparison in [83] reveals an artifact of Feynman's approach where in the intermediate coupling regime the effective mass rapidly jumps nearly an order of magnitude and provides an extremely sharp transition to the strong coupling regime as shown in Figure 2.6. In this part we show that in the general memory kernel approach this artifact disappears and the transition is smoothed out. Although the effective mass in the general memory kernel approach in the context of the optical Fröhlich polaron has been rigorously derived in [87], here we will follow the simple trick proposed by Feynman [8] in the limit of low velocities. Although the trick might appear somewhat informal it has been shown to be equivalent with more rigorous derivations [88]. We imagine a velocity boost \mathbf{v} on the impurity, which corresponds to the following transformation in the interaction terms of both the effective and model actions:

$$\mathbf{r}(\tau) - \mathbf{r}(\sigma) \to \mathbf{r}(\tau) - \mathbf{r}(\sigma) - \mathbf{v}(\tau - \sigma).$$
 (2.25)

The goal is now to once again derive the variational free energy $F_v(\mathbf{v})$ after

this boost and to expand this expression up to second order in \mathbf{v} at small velocities. The factor appearing in front of the second order term $\sim \mathbf{v}^2/2$ then physically represents the role of an effective mass at small velocities. It can be easily deduced from [87] that in the two terms related to the model action: $F_0 - \frac{1}{\beta} \langle S_0 \rangle$, the second order contribution in the velocity will simply correspond to a kinetic energy term with the bare mass of the impurity $\sim m\mathbf{v}^2/2$. Consequently, to obtain the effective mass correction on top of the bare impurity mass m, all we have to compute is the following boosted expectation value:

$$\langle S_{\text{eff}} \rangle_0 \left(\mathbf{v} \right) = -\frac{1}{V} \sum_{\mathbf{k}} \frac{g_{ib}^2 n_0}{2\hbar} V_{\mathbf{k}}^2 \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma \mathcal{G} \left(\mathbf{k}, |\tau - \sigma| \right) \mathcal{F}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{v}(\tau - \sigma)} \quad (2.26)$$

and then identify its second order expansion term in **v**. Expression (2.26) is clearly a function of $|\tau - \sigma|$ as changing a sign in the exponential can be lifted by merely renaming $\mathbf{k} \to -\mathbf{k}$ and obtaining an identical expression. For any such function one can transform into the center of mass and relative coordinates of τ and σ to show:

$$\int_0^\beta d\tau \int_0^\beta d\sigma f(|\tau - \sigma|) = 2 \int_0^\beta (\beta - u) f(u) du.$$
(2.27)

If this formula is applied to (2.26), for $u \to \infty$ the oscillation term will make the function f(u) dampen out to zero, and we can therefore assume that the function f(u) goes to zero at large u. Since we will be dividing (2.26) by an additional β to get the correction in the free energy, we can drop the second term of the integrand in (2.27) at zero temperature and use the identity:

$$\int_0^\beta d\tau \int_0^\beta d\sigma f(|\tau - \sigma|) = 2\beta \int_0^\infty f(u)du \qquad (2.28)$$

to find in this limit:

$$\frac{1}{\beta} \langle S_{\text{eff}} \rangle_0 \left(\mathbf{v} \right) = -\frac{1}{V} \sum_{\mathbf{k}} g_{ib}^2 n_0 \ V_{\mathbf{k}}^2 \int_0^\beta du \mathcal{G} \left(\mathbf{k}, u \right) \mathcal{F}_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{v} u}.$$
(2.29)

The second-order contribution of this expectation value is now given by

$$\delta F_{\mathbf{v}^2} = \frac{1}{2V} \sum_{\mathbf{k}} g_{ib}^2 n_0 \ V_{\mathbf{k}}^2 \int_0^\beta du \mathcal{G}\left(\mathbf{k}, u\right) \mathcal{F}_{\mathbf{k}} \left(\mathbf{k} \cdot \mathbf{v}\right)^2 u^2, \tag{2.30}$$



FIGURE 2.6: The effective polaron mass m_{eff} at cutoff $\Lambda = 200\xi^{-1}$ computed with Feynman's original model (dashed green), the general memory kernel model (solid blue), the extended RG approach (red circles) [83] and the Landau-Pekar strong coupling results from [68].

where following identity for any d-dimensional integral of this form:

$$\int \mathbf{d}\mathbf{k}^d f(k) (\mathbf{k} \cdot \mathbf{v})^2 = \frac{1}{d} \int \mathbf{d}\mathbf{k} f(k) k^2 v^2$$
(2.31)

can now be used to write

$$\delta F_{\mathbf{v}^2} = \mathbf{v}^2 \frac{1}{V} \frac{1}{6} \sum_{\mathbf{k}} g_{ib}^2 n_0 \ V_{\mathbf{k}}^2 \int_0^\beta du \mathcal{G}(\mathbf{k}, u) \ \mathcal{F}_{\mathbf{k}} k^2 u^2.$$
(2.32)

Finally, the effective mass of the polaron is given by:

$$m_{\rm eff} = m + \frac{1}{V} \frac{1}{3} \sum_{\mathbf{k}} g_{ib}^2 n_0 \ V_{\mathbf{k}}^2 \int_0^\beta du \mathcal{G}(\mathbf{k}, u) \ \mathcal{F}_{\mathbf{k}} k^2 u^2, \tag{2.33}$$

which in polaronic units yields:

$$m_{\text{eff}} = m + \frac{\alpha}{12\pi\mu^2} \int dk k^4 V_{\mathbf{k}}^2 \int_0^\infty du \mathcal{G}\left(\mathbf{k}, u\right) \mathcal{F}_{\mathbf{k}} u^2.$$
(2.34)

The result is presented at a cutoff of $\Lambda = 200\xi^{-1}$ in Figure 2.6 to compare with the extended RG approach. We can see that the main artifact of Feynman's approach is lifted in the general memory kernel method and the transition from the weak to strong coupling regimes is smoothed out. Nevertheless, a noticeable

discrepancy remains between our approach and RG going into the strong coupling regime. Although the RG approach has been shown to be in good agreement with diagMC for the ground state energy, we are not aware of any diagrammatic nor experimental result for the effective mass of the Bogoliubov-Fröhlich model that could be used as a gauge and hence the remaining discrepancy between the two methods cannot be unanimously addressed.

Some observations favorable towards the general memory kernel result can be made. Although no formal guarantee exists, it is reasonable to expect that improving the model action from Feynman's approach to the general memory kernel formalism should also improve the accuracy of the effective mass. At intermediate coupling around $\alpha \approx 1.5$ in Figure 2.6 the general kernel result for the effective mass shifts closer towards RG, as would be expected. However, at stronger coupling around $\alpha = 5$ the improved approach shifts the result *farther* away from RG. On the premise that improving the model action in the variational formalism also improves the result for the effective we therefore have indications that the RG approach might be underestimating the effective mass at strong coupling.

2.5 Second order correction

In Section 2.3 we have shown that improving the model action to the general memory kernel form already yields good agreement with diagMC at strong coupling. However, as we will see in this section, this turns out to be insufficient at intermediate coupling and hence the goal is to obtain even further corrections. By adding and subtracting the model action functional S_0 in the path integral of the polaron partition function (2.1), the free energy of the system can be exactly written as [89]:

$$F = F_0 - \frac{1}{\beta} \ln\left(\left\langle e^{-\Delta S} \right\rangle\right), \qquad (2.35)$$

where $\Delta S = S_{\text{eff}} - S_0$, and the expectation values are taken with respect to the model action. The second term can be recognized as the cumulant-generating function of the path integral, which can be expanded as [78, 89]

$$F = F_0 + \frac{1}{\beta} \left\langle \Delta \mathcal{S} \right\rangle_0 - \frac{1}{2!} \frac{1}{\beta} \left\langle \left(\Delta \mathcal{S} - \left\langle \Delta \mathcal{S} \right\rangle \right)^2 \right\rangle + \mathcal{O} \left(\Delta \mathcal{S}^3 \right).$$
(2.36)

Here, we can recognize the variational free energy in the first two terms, which represent the Jensen-Feynman inequality (2.4) if all the higher order terms are discarded.

In this section we perturbatively include the second order correction in the cumulant expansion of (2.36). This correction has been studied and shown to be small in the Fröhlich model [78, 79], but we find it to be non-negligible in the Bogoliubiov-Fröhlich model. We emphasize that the resulting correction is approximate for two reasons. First of all to the best of our knowledge, no general inequalities that include higher orders of the expansion are known [90] and hence from this point on the variational inequality can be violated. Second, the obtained correction is significantly more difficult to compute than the one obtained in [79] due to the fact that the momentum integrals cannot be analytically performed in the Bogoliubov-Fröhlich model. For this reason a mean-field like approximation to obtain a semi-analytic expression will be made. At weak to intermediate coupling the obtained corrected energy is in excellent agreement with diagMC and exhibits the exact logarithmic divergence that was observed in [10].

In what follows we are strictly interested in the $\beta \to \infty$ limit. For convenience of notation, and to avoid having to write the formal limit everywhere, we will keep the Matsubara summations in their discrete form and still write the factor β in e.g. the integral boundaries. Such expressions are to be strictly interpreted on the condition that β is very large and will be taken to infinity in the end, on which our derivation relies. The cumulant in the second order correction can be written as:

$$\frac{1}{2\beta} \left\langle (\Delta S - \langle \Delta S \rangle)^2 \right\rangle = \frac{1}{2\beta} \left[\left\langle \tilde{S}_{\text{eff}}^2 \right\rangle - \left\langle \tilde{S}_{\text{eff}} \right\rangle^2 \right] \\
+ \frac{1}{2\beta} \left[\left\langle \tilde{S}_0^2 \right\rangle - \left\langle \tilde{S}_0 \right\rangle^2 \right] - \frac{1}{\beta} \left[\left\langle \tilde{S}_{\text{eff}} \tilde{S}_0 \right\rangle - \left\langle \tilde{S}_{\text{eff}} \right\rangle \left\langle \tilde{S}_0 \right\rangle \right].$$
(2.37)

In Appendix (A) we show that if the following fivefold integral is defined:

$$\sigma_{n}[x(\nu)] = \frac{1}{(2n+1)!} \left(\frac{\alpha}{4\pi\mu^{2}}\right)^{2} \int_{0}^{\Lambda} dk \int_{0}^{\Lambda} ds k^{2} s^{2} V_{\mathbf{k}}^{2} V_{\mathbf{s}}^{2} \times \int_{0}^{\beta/2} du_{1} \int_{0}^{\beta/2} du_{2} \mathcal{G}_{\mathbf{k}}(u_{1}) \mathcal{G}_{\mathbf{s}}(u_{2}) \mathcal{F}_{\mathbf{k}}(u_{1}) \mathcal{F}_{\mathbf{s}}(u_{2}) \int_{0}^{\beta/2} dz \left(\frac{ks}{4} \zeta(u_{1}, u_{2}, z)\right)^{2n},$$
(2.38)

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where:

$$\zeta(u_1, u_2, z) = \frac{32}{\beta} \sum_{n=1}^{\infty} \left[\frac{1}{\nu_n^2 + x_n} \cos(\nu_n z) \sin\left(\frac{\nu_n u_1}{2}\right) \sin\left(\frac{\nu_n u_2}{2}\right) \right], \quad (2.39)$$

for any memory kernel $x(\nu)$, the second order correction (2.37) can be written as:

$$\frac{1}{2\beta} \left\langle \left(\Delta \mathcal{S} - \left\langle \Delta \mathcal{S} \right\rangle\right)^2 \right\rangle = \sum_{n=2}^{\infty} \sigma_n[x(\nu)] + \left[\sigma_1[x(\nu)] + \frac{1}{2\beta} \left(\left\langle \tilde{\mathcal{S}}_0^2 \right\rangle - \left\langle \tilde{\mathcal{S}}_0 \right\rangle^2 \right) - \frac{1}{\beta} \left(\left\langle \tilde{\mathcal{S}}_{\text{eff}} \tilde{\mathcal{S}}_0 \right\rangle - \left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle \left\langle \tilde{\mathcal{S}}_0 \right\rangle \right)\right].$$
(2.40)

Note that if $x(\nu) = 0$ is substituted in the variational free energy (2.23) one obtains the mean-field Lee-Low-Pines result at zero polaron momentum. Therefore, for $x(\nu) = 0$ we can interpret the result (2.40) as a correction to mean-field theory:

$$\frac{1}{2\beta} \left\langle \left(\Delta S - \left\langle \Delta S \right\rangle\right)^2 \right\rangle^{(\mathrm{MF})} = \sum_{n=1}^{\infty} \sigma_n[0].$$
(2.41)

Incidentally, the polaron problem mean-field theory corresponds to first-order perturbation theory [57], and hence (2.41) is also nothing else than the second order perturbative correction. Due to the simplification $x(\nu) = 0$, the sum in (2.41) can be performed. However, mean-field theory completely misses the diagMC polaronic energy in the Bogoliubov-Fröhlich Hamiltonian beyond weak coupling as illustrated in Figure 2.2 and hence it is desirable to start from a better point.

Let us now consider the corrections on top of the best quadratic action functional with the optimized memory kernel (2.24). As shown in Appendix (A), in this case the terms in the square brackets in (2.40) all completely cancel and the summation starts from n = 2

$$\frac{1}{2\beta} \left\langle \left(\Delta \mathcal{S} - \left\langle \Delta \mathcal{S} \right\rangle\right)^2 \right\rangle^{\text{(best)}} = \sum_{n=2}^{\infty} \sigma_n[x(\nu)].$$
(2.42)

Therefore an important feature of expanding around the best quadratic action is to omit the dominant contribution from σ_1 in the mean-field correction (2.41). In contrast with previous approaches that have considered the second order correction for the polaron, the momentum integrals in (2.38) cannot be performed analytically. For any non-trivial memory kernel $x(\nu)$ one is hence left with a fivefold integral, which we have not been able to compute efficiently.

Let us therefore in spirit of Feynman's approach consider a simple semi-analytic

approximation. We expand around the best quadratic action in (2.40) and use this knowledge to cancel the term in the square brackets, but then approximate the remaining contributions at the mean-field level:

$$\frac{1}{2\beta} \left\langle (\Delta S - \langle \Delta S \rangle)^2 \right\rangle^{\text{(best)}} \approx \sum_{n=2}^{\infty} \sigma_n[0].$$
(2.43)

The error of this approximation is roughly estimated by calculating the difference in the first-order term $\sigma_1[x(\nu)] - \sigma_1[0]$, which is the only exception for which the fivefold integral can be rather easily performed. This difference is obtained in expression (A.21) in Appendix (A) (which is to be computed in the $\beta \to \infty$ limit):

$$\sigma_1[x(\nu)] - \sigma_1[0] = \frac{3}{2\beta} \sum_{n=1}^{\infty} \left[\frac{x_n^2}{(\nu_n^2 + x_n)^2} - \frac{\tilde{x}_n^2}{\nu_n^4} \right].$$
(2.44)

Here, x_n represents the optimal memory kernel, whereas \tilde{x}_n is the first-order iterative improvement obtained from substituting $x(\nu) = 0$ into (2.24). For a cutoff $\Lambda = 2000\xi^{-1}$ the relative error on the correction is of the order of 3% for $\alpha = 0.5$ and of the order of 5% for $\alpha = 1$. This justifies using the approximation to get an accurate second order correction in the weak to intermediate coupling regime, in particular for Figure 2.7. This error is however larger at large coupling strengths, and we found an over correction towards energies below diagMC for $\alpha > 5$ when applied to Figure 2.3. This suggests that even higher order corrections are likely needed to get exactly on diagMC in that regime, and in what follows we only apply the correction in the weak to intermediate coupling regime.

As shown in Appendix (B), the full corrected energy on top of the minimized E_v from (2.23), with this approximated correction is given by:

$$E = E_v - \alpha^2 Q, \qquad (2.45)$$

where:

$$Q = \sum_{n=2}^{\infty} \frac{1}{(2n+1)} \left(\frac{1}{4\pi\mu^2}\right)^2 \int_{0}^{\Lambda} dk \int_{0}^{\Lambda} ds V_{\mathbf{k}}^2 V_{\mathbf{s}}^2 \frac{k^{2+2n} s^{2+2n} \left(3a(k) + a(s)\right)}{a(k)^2 \left(a(k) + a(s)\right)^{2+2n}}, \quad (2.46)$$

with $a(k) = \omega_k + k^2/(2m)$. This double integral can be readily performed and the series converges within less than 0.1% after n = 10. If the sum is extended to n = 0, the series expansion of $x \arctan(x)$ can be recognized here which indicates



FIGURE 2.7: The polaronic energy obtained from diagrammatic Monte Carlo [10] (squares with error bars) at $\Lambda = 2000\xi^{-1}$ is compared to the result of Feynman's original model action (dashed curve), to the result of the general memory kernel method of Sec. 2.3 (dashdotted curve), and to the general memory kernel result including the second order correction of Sec. 2.5 (solid curve).

that the integral could likely be more easily performed in the $\sinh(x)/x$ form in (A.13) once the $x(\nu) = 0$ approximation is made. Nevertheless, the series expansion proves to be useful to discuss the differences of the corrections in (2.41) and (2.42).



FIGURE 2.8: The polaronic energy contribution obtained within Feynman's original model (dashed), the general memory kernel method (dashdotted) and the corrected energy (solid) with diagrammatic Monte Carlo [10] (squares) are plotted for $\alpha = 3$ as a function of the cutoff Λ on a logarithmic scale.

In Figure 2.7 we compare the results with diagMC values obtained at small to intermediate coupling strengths [10] at a cutoff of $\Lambda = 2000\xi^{-1}$. We see that a significant correction to Feynman's original model is obtained by using the general memory kernel method, but nevertheless in the challenging intermediate coupling regime noticeable discrepancies remain. The corrected energy to second order discussed in this section yields excellent agreement with diagMC in this regime. It should be emphasized that both the RG [68] and CGW [64] methods yield equally good agreement with diagMC here.

Finally, in Figure 2.8 we show how the logarithmic divergence observed in diagMC can be completely retrieved in the corrected energy. Once again, while the general memory kernel approach yields significant improvements to the original model system, the corrected energy is necessary to obtain further agreement with diagMC. However, it should be noted that in this regime at $\alpha \approx 3$, especially at small cutoff values, we leave the weak to intermediate coupling regime and the

Bogoliubov-Fröhlich Hamiltonian at large cutoff $\Lambda \approx 2000 - 3000\xi^{-1}$				
Coupling regime	$\alpha < 0.1$	$\alpha \approx 1$	$\alpha \approx 10$	log-div?
Mean field	\checkmark	×	Х	×
Feynman	\checkmark	×	×	×
CGW	\checkmark	\checkmark	×	\approx
perturbative RG	\checkmark	\checkmark	×	\approx
extended RG	\checkmark	\checkmark	\checkmark	\checkmark
(new) General memory	\checkmark	\approx	\checkmark	\approx
		\downarrow		\downarrow
(new) Correction		\checkmark		\checkmark

TABLE 2.1: A qualitative comparison between the different theoretical approaches to the ground state energy of the Bogoliubov-Fröhlich Hamiltonian as compared to diagMC. Rough estimators: (\checkmark) indicates good agreement with diagMC, (\times) indicates significant discrepancy, and (\approx) indicates some discrepancy from diagMC. The last two entries correspond to the methods developed in this chapter where the arrows indicate a correction at intermediate coupling strengths.

approximation (2.43) can no longer be safely justified to accurately represent the second order cumulant correction. Nevertheless, the expression appears to be in excellent agreement with diagMC, but we leave open the possibility that the exact second order correction would slightly overcorrect diagMC in this regime, to be only brought back in the third order cumulant. Neglecting this caveat, we note that the result obtained in Figure 2.8 is in better agreement with diagMC than either perturbative RG or CGW that only capture the slope of the divergence correctly but are shifted by an appreciable energy as shown in Figure 2.2. A comparison with the extended RG method in this regime cannot be made since this graph was not presented in [83], but based on the other results in the paper it is expected that extended RG should be accurate here as well.

In Table 2.1 we present a comparison between the different methods, where we emphasize that the labels are estimated qualitatively. We conclude that with the inclusion of the higher order correction, the method developed in this chapter compares better to diagMC than the two other extensively used approaches in the literature in the last years: CGW and perturbative RG, and is comparable to the more recent extended RG approaches. This is in particular noticeable at either strong coupling or in the logarithmic divergence plot in Figure 2.8. Our approach has one disadvantage worth mentioning – the second order correction is perturbative in nature and is computed within an additional mean-field approximation. As demonstrated, this works well in the weak to intermediate coupling regime at large cutoff. However, at strong coupling, roughly starting at $\alpha > 5$ the perturbative term yields an overcorrection of the energy and the obtained result drops slightly below diagMC. This overcorrection is not large but nevertheless indicates that the upper bound of the variational approach is lost.

On the other hand, our approach has a couple of nice properties. First of all, thermal fluctuations of the impurity and phonons, or the presence of multiple impurities, could be taken into account without any fundamental changes. It is not clear how feasible this is in the other approaches in the literature. In addition it is completely transparent at this point where the remaining corrections to our approach are situated:

- The exact second order correction can be obtained by finding an efficient way to compute the fivefold integral in (2.38).
- Any remaining discrepancies are guaranteed to be situated in the higher order cumulant terms $\mathcal{O}(\Delta S^3)$. Since we have presented a way to approximate the second order correction here, perhaps the difficult higher order corrections could be dealt with in a similar way. It would be interesting to see whether a full series resummation of all the corrections can be obtained at this approximate level.

We leave these questions open for future studies.

2.6 Conclusion

In conclusion, in this chapter we explored extensions of Feynman's variational path integral treatment of the Bogoliubov-Fröhlich model and addressed the issues of this method that were brought up in a number of works [10, 64, 68]. The main message of this chapter is that the variational path integral approach can be improved to be of comparable or better accuracy as other modern theoretical tools that were recently employed to study the difficult Bose polaron problem. We show that two adjustments can be made to obtain major improvements to the original approach to this model that was first studied in [48].

First, instead of considering a coupled oscillator for the model action, a general quadratic action functional with a variational memory kernel is proposed. This method has already been studied for the original Fröhlich model [76, 77] but

was found to yield only minor corrections. We show that this step is absolutely necessary to treat the Bogoliubov-Fröhlich model, and obtain relatively good agreement with diagMC at strong coupling.

To capture the difficult intermediate regime where the phonons of the model are strongly correlated [64], even with this improvement noticeable discrepancies remain. For this reason we propose to include higher order corrections to the energy beyond the first order variational inequality, expanded around the general model action functional. These corrections have also been studied in the context of the original Fröhlich model [78, 79, 89], but the studies were situated strictly within Feynman's approach and in addition the corrections were found to be small. In this chapter we have generalized previous results to the general memory kernel case and applied it to the Bogoliubov-Fröhlich model. To obtain an easy semi-analytic expression for the correction we have proposed an approximation that naturally presents itself within the general memory kernel treatment. We estimated this approximation to be accurate in the weak to intermediate coupling regime and obtain excellent agreement with diagMC. In addition, the correct logarithmic divergence of the model is retrieved. Renormalization procedures of the divergence are discussed in [56, 68]

This approach could be extended to many particles or to finite temperatures, which could be a way to probe the effect of thermal fluctuations on a system where quantum fluctuations are of great importance. Having seen how the second order correction around the optimal quadratic action functional can be approximated by subtracting a single term from the perturbative correction with respect to a free particle, it would also be interesting to explore this in the context of higher order corrections.

CHAPTER 3

The path integral approach for the extended Fröhlich model

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In this chapter we will use the path integral approach to tackle the extended Fröhlich Hamiltonian (1.26) introduced in Chapter 1. The focus will lie on understanding the effect of the extended interactions on the polaron ground state properties such as the ground state energy, effective mass and polaron radius. For this reason, extensive comparison to the Fröhlich model will be made. In the process we will encounter a problem of a completely different nature than in the previous chapter. For the Fröhlich model, which has been studied in Chapter 2, the effective action of the polaron \mathcal{S}_{eff} is exactly known and the problem lies in variationally capturing its physics by improving the model action \mathcal{S}_0 . However, for the extended Bogoliubov-Fröhlich model, obtaining the effective action \mathcal{S}_{eff} forms a significantly more difficult problem that was yet unsolved in the literature at the moment of this study. In this chapter, our efforts will therefore be directed towards finding a framework to obtain \mathcal{S}_{eff} of the extended Fröhlich model. In contrast to the previous chapter, the resulting expression for the extended action will be treated within Feynman's original model action as most of the effects of the extended interactions can already be qualitatively captured at this level.

Chapter 3 - The path integral approach for the extended Fröhlich model

3.1 The extended action functional

We remind the reader that for a single particle immersed in a Bose-Einstein condensate the extended Fröhlich Hamiltonian, introduced in (1.26) of Chapter 1, is given by:

$$\hat{H}_{EF} = \frac{\hat{\mathbf{p}}^2}{2m} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}^{\dagger}_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} + \frac{g_{ib}\sqrt{N_0}}{V} \sum_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}^{\dagger}_{-\mathbf{k}} \right) + \frac{g_{ib}}{V} \sum_{\mathbf{s}\neq\mathbf{0}} \sum_{\mathbf{k}\neq\mathbf{0}} \hat{\rho}_{\mathbf{k}-\mathbf{s}} W^{(1)}_{\mathbf{k},\mathbf{s}} \hat{\alpha}^{\dagger}_{\mathbf{s}} \hat{\alpha}_{\mathbf{k}} + \frac{1}{2} \frac{g_{ib}}{V} \sum_{\mathbf{s}\neq\mathbf{0}} \sum_{\mathbf{k}\neq\mathbf{0}} \hat{\rho}_{\mathbf{k}-\mathbf{s}} W^{(2)}_{\mathbf{k},\mathbf{s}} \left(\hat{\alpha}^{\dagger}_{\mathbf{s}} \hat{\alpha}^{\dagger}_{-\mathbf{k}} + \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{-\mathbf{s}} \right). \quad (3.1)$$

Here, the first line corresponds to the thoroughly discussed Bogoliubov-Fröhlich Hamiltonian of the previous chapter and the second line consists of the extended terms with respect to the Fröhlich Hamiltonian with the two new interaction amplitudes:

$$W_{\mathbf{k},\mathbf{k}'}^{(1)} = \frac{1}{2} \left(V_{\mathbf{k}} V_{\mathbf{k}'} + V_{\mathbf{k}}^{-1} V_{\mathbf{k}'}^{-1} \right), \qquad (3.2)$$

$$W_{\mathbf{k},\mathbf{k}'}^{(2)} = \frac{1}{2} \left(V_{\mathbf{k}} V_{\mathbf{k}'} - V_{\mathbf{k}}^{-1} V_{\mathbf{k}'}^{-1} \right).$$
(3.3)

This extended Hamiltonian provides a correction to the Bogoliubov-Fröhlich model by taking into account events where an impurity is interacting with two excitation operators at once without direct coupling to the condensed state. These terms allow for processes where an excitation of the condensate scatters off the impurity multiple times before being absorbed.

To treat the Hamiltonian within the path integral formalism, first an expression for its action functional S_{tot} has to be found. This step can be seen as moving in the opposite direction of quantizing a theory with the goal of obtaining a classical description of the Hamiltonian (3.1). By following the same reasoning as Feynman initially did to obtain the effective action of the Fröhlich model [62], we derive the following extended Fröhlich Lagrangian in Appendix (C):

$$L = \frac{m\dot{\mathbf{r}}^2}{2} + \frac{M}{2} \sum_{\mathbf{k}} \dot{Q}_{\mathbf{k}} \dot{Q}_{-\mathbf{k}} - \sum_{\mathbf{k}} \frac{M\omega_{\mathbf{k}}^2}{2} Q_{-\mathbf{k}} Q_{\mathbf{k}} - \frac{\sqrt{N_0} g_{ib}}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \rho_{\mathbf{k}} \sqrt{\frac{2M\omega_{\mathbf{k}}}{\hbar}} V_{\mathbf{k}} Q_{\mathbf{k}} - \frac{g_{ib}}{V} \frac{M}{2} \sum_{\mathbf{k},\mathbf{s}} \rho_{\mathbf{k}-\mathbf{s}} V_{\mathbf{k}} V_{\mathbf{s}} \frac{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}}{\hbar} Q_{-\mathbf{s}} Q_{\mathbf{k}} - \frac{g_{ib}}{V} \frac{M\eta}{2} \sum_{\mathbf{k},\mathbf{s}} \frac{V_{\mathbf{k}}^{-1} V_{\mathbf{s}}^{-1}}{\hbar\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}} \rho_{\mathbf{k}-\mathbf{s}} \dot{Q}_{\mathbf{k}} \dot{Q}_{-\mathbf{s}}.$$

$$(3.4)$$
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where:

$$\eta = \left(1 + \frac{g_{ib}}{V} \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{-2}}{\hbar\omega_{\mathbf{k}}}\right)^{-1}$$
(3.5)

vanishes at infinite cutoff if no regularization procedures of the contact interactions are performed. The variables $Q_{\mathbf{k}}^* = Q_{-\mathbf{k}}$ are now scalars suitable for path integration. The first four terms of (3.4) correspond to the Lagrangian of the Fröhlich model and yield the Fröhlich action \mathcal{S}^F as given in (1.47). The additional terms in (3.4) take into account the extended interactions beyond the Fröhlich model and consist of a part depending on the phonon coordinates $Q_{\mathbf{k}}$ multiplied by $V_{\mathbf{k}}$, and a part depending on the phonon velocities $\dot{Q}_{\mathbf{k}}$ along with $V_{\mathbf{k}}^{-1}$. Within a mean-field approach where the excitation operators acquire a polaronic shift $\hat{\alpha}_{\mathbf{k}} \rightarrow \hat{\alpha}_{\mathbf{k}} - f_{\mathbf{k}}$, these velocity-dependent terms can be shown to arise due to a non-zero imaginary contribution from $f_{\mathbf{k}}$ and vanish for the saddle-point solution at rest [50, 59], while the terms containing $V_{\mathbf{k}}$ arise due to the real part of $f_{\mathbf{k}}$ and have a non-negligible contribution to the ground-state energy resulting in a resonance shift. In the RG approach [70] it is pointed out that the RG coupling constant corresponding to the $V_{\mathbf{k}}^{-1}$ terms has a small effect on the polaron wavefunction, but is expected to be important when considering other qualitative properties such as the lifetime of the polaron due to the appearance of bound states at lower energies. These considerations are, however, beyond the scope of the goals of this chapter and we will only consider the position-dependent terms of the extended interactions. In this way we capture the same effects as the mean-field treatment but treat them beyond the mean-field level. Hence, in the remainder of this chapter, we consider the Euclidean polaron action functional,

$$S = S^{F} + \frac{g_{ib}}{V} \frac{M}{2} \sum_{\mathbf{k},\mathbf{s}} \int_{0}^{\hbar\beta} d\tau \rho_{\mathbf{k}-\mathbf{s}}(\tau) V_{\mathbf{k}} V_{\mathbf{s}} \frac{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}}{\hbar} Q_{\mathbf{s}}^{*}(\tau) Q_{\mathbf{k}}(\tau), \qquad (3.6)$$

where

$$S^{F} = \int_{0}^{\hbar\beta} \left(\frac{m \dot{\mathbf{r}}^{2}}{2} + \frac{M}{2} \sum_{\mathbf{k}} \dot{Q}_{\mathbf{k}}^{*} \dot{Q}_{\mathbf{k}} + \sum_{\mathbf{k}} \frac{M \omega_{\mathbf{k}}^{2}}{2} Q_{\mathbf{k}}^{*} Q_{\mathbf{k}} + \frac{\sqrt{N_{0}} g_{ib}}{V} \sum_{\mathbf{k}} \rho_{\mathbf{k}} \sqrt{\frac{2M \omega_{\mathbf{k}}}{\hbar}} V_{\mathbf{k}} Q_{\mathbf{k}} \right) d\tau$$

$$(3.7)$$

is the action of the Fröhlich model.

3.2 Perturbative expansion for the beyond Fröhlich terms

The goal of this subsection is to integrate out the phonon variables $Q_{\mathbf{k}}$ and obtain the effective action \mathcal{S}_{eff} action corresponding to (3.6):

$$e^{-\mathcal{S}_{\text{eff}}/\hbar} = \int \mathcal{D}\{Q_{\mathbf{k}}\} \exp\left(-\frac{g_{ib}}{V}\frac{M}{2}\sum_{\mathbf{k},\mathbf{s}} V_{\mathbf{k}}V_{\mathbf{s}}\frac{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}}{\hbar^{2}}\int_{0}^{\hbar\beta} d\tau \rho_{\mathbf{k}-\mathbf{s}}(\tau)Q_{\mathbf{k}}(\tau)Q_{\mathbf{s}}^{*}(\tau)\right) e^{-\mathcal{S}^{F}/\hbar}.$$
(3.8)

Within the Fröhlich model this path integral corresponds to a driven harmonic oscillator and is readily solved. However, to the best of our knowledge, the type of path integral in presence of off-diagonal extended terms $Q_{\rm s}^*(\tau)Q_{\rm k}(\tau)$ has not yet been encountered in the literature at the moment of study. In what follows, we propose a strategy to find a solution by expanding the extended terms in a perturbative series and search for patterns in the resulting terms. The efficacy of this initial approach presented here has also motivated the development of a more recent systematic treatment of this path integral in the context of the solid state polaron in the presence of anharmonic interactions [91].

The idea is to take into account the exponential of the beyond-Fröhlich terms in (3.8) perturbatively through a series expansion of the exponential and a subsequent integration over the phonon degrees of freedom. The terms in the resulting perturbation series can be obtained more straightforwardly with the generating functional formalism. The generating functional is obtained by adding source terms (and a prefactor that will simplify the algebra) to the Fröhlich action:

$$S^{F}[J_{\mathbf{k}}] = S^{F} + \frac{1}{2} \frac{\sqrt{N_{0}} g_{ib}}{V} \int_{0}^{\hbar\beta} \sum_{\mathbf{k}} \sqrt{\frac{2M\omega_{\mathbf{k}}}{\hbar}} V_{\mathbf{k}} \left[Q_{\mathbf{k}}(\tau) J_{\mathbf{k}}(\tau) + Q_{\mathbf{k}}^{*}(\tau) J_{\mathbf{k}}^{*}(\tau) \right] d\tau.$$

$$(3.9)$$

The source terms resemble the Fröhlich impurity-phonon interaction term, and can be added to it. Hence, including the source terms in the Fröhlich action amounts to shifting $\rho_{\mathbf{k}}$ to $\rho_{\mathbf{k}} + J_{\mathbf{k}}$. The generating functional is then obtained by integrating out the phonon degrees of freedom. The resulting effective action of the Fröhlich model including source terms then becomes:

$$S_{\text{eff}}^{F}[J_{\mathbf{k}}] = \int_{0}^{\hbar\beta} \frac{m\dot{\mathbf{r}}^{2}}{2} dt - \sum_{\mathbf{k}} \frac{g_{ib}^{2}n_{0}}{2\hbar V} V_{\mathbf{k}}^{2} \\ \times \int_{0}^{\hbar\beta} d\tau \int_{0}^{\hbar\beta} d\sigma \mathcal{G}_{\mathbf{k}}(\tau - \sigma) \left[\rho_{\mathbf{k}}(\tau) + J_{\mathbf{k}}(\tau)\right] \left[\rho_{\mathbf{k}}^{*}(\sigma) + J_{\mathbf{k}}^{*}(\sigma)\right].$$
(3.10)

In the series expansion of the exponential in (3.8) the phonon position variables $Q_{\mathbf{k}}$ can be replaced by functional derivatives with respect to $J_{\mathbf{k}}$, which can be brought out of the functional integral over $Q_{\mathbf{k}}$. After performing the path integral over the phonon variables one is left with the following expression:

$$e^{-\mathcal{S}_{\text{eff}}/\hbar} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left[\frac{\hbar}{g_{ib}n_0} \sum_{\mathbf{k},\mathbf{s}} \int_0^{\hbar\beta} d\tau \rho_{\mathbf{k}-\mathbf{s}}(\tau) \frac{\delta}{\delta J_{\mathbf{k}}(\tau)} \frac{\delta}{\delta J_{\mathbf{s}}^*(\tau)} \right]^n e^{-\mathcal{S}_{\text{eff}}^F[J_{\mathbf{k}}]/\hbar} \bigg|_{J_{\mathbf{k}}=0}$$
(3.11)

We will now provide an overview of the structure of the various terms appearing in the generating functional series (3.11) and argue which terms can be neglected. They can be classified in three categories.

3.2.1 VACUUM ENERGY TERMS

It is illustrative to consider the n = 1 order in the expansion. After the first $\frac{\delta}{\delta J_{\mathbf{s}}^*(\tau)}$ in (3.11) is applied to the exponential, one obtains

$$e^{-\mathcal{S}_{\text{eff}}/\hbar} = \left[1 - \frac{g_{ib}}{2\hbar V} \sum_{\mathbf{k},\mathbf{s}} V_{\mathbf{s}}^2 \int_0^{\hbar\beta} d\tau \rho_{\mathbf{k}-\mathbf{s}}(\tau) \frac{\delta}{\delta J_{\mathbf{k}}(\tau)} \right]$$
$$\int_0^{\hbar\beta} \mathcal{G}_{\mathbf{s}}(\tau - \sigma) \left[\rho_{\mathbf{s}}(\sigma) + J_{\mathbf{s}}(\sigma) \right] d\sigma \left[e^{-\mathcal{S}_{\text{eff}}^F[J_{\mathbf{k}}]/\hbar} \right]_{J_{\mathbf{k}}=0}.$$
(3.12)

Now, there is a choice whether to apply the second operator $\frac{\delta}{\delta J_{\mathbf{k}}(\tau)}$ to the exponential again or to the $J_{\mathbf{s}}(t)$ in front. The former option leads to terms which will be discussed in the next subsection. The latter option fully eliminates the impurity variable and results in:

$$e^{-\mathcal{S}_{\text{eff}}/\hbar} = \left[1 - \frac{g_{ib}\beta}{2V} \sum_{\mathbf{k}} V_{\mathbf{k}}^2 \mathcal{G}(\mathbf{k}, 0)\right] e^{-\mathcal{S}_{\text{eff}}^F[J_{\mathbf{k}}]/\hbar} \Big|_{J_{\mathbf{k}}=0}.$$
 (3.13)

In every order n of the expansion there will be $0 \le j \le n$ operator pairs in which each individual pair is applied in the same way as in this example to eliminate the impurity variable and merely yield the term in (3.13) to the power j multiplied with a combinatorial factor. This allows to separate these terms and perform their complete series summation, given that they are not to be counted from this point on. The summation results in the following contribution to the effective action:

$$\delta S_{\text{eff}} = \frac{g_{ib}\hbar\beta}{2V} \sum_{\mathbf{k}} V_{\mathbf{k}}^2 \mathcal{G}(\mathbf{k}, 0).$$
(3.14)

At zero temperature the corresponding energy shift is given by:

$$\Delta E_{vac} = \frac{g_{ib}}{2V} \sum_{\mathbf{k}} V_{\mathbf{k}}^2. \tag{3.15}$$

This contribution is precisely of the same type as the divergent terms arising from non-commuting variables in the derivation of the Lagrangian (3.4). First-order corrections in g_{ib} to the ground-state energy are not observed in a rigorous perturbative calculation [92] and we do not expect these terms to be of physical significance. Furthermore note that (3.15) is UV divergent and can not be regularized by taking the cutoff dependence of g_{ib} into account. Therefore we will discard contribution (3.14) in the rest of our calculations.

3.2.2 Scattering terms

In the previous example of expansion order n = 1 we could have also applied the second functional derivative to the exponential again in (3.12) to find:

$$e^{-\mathcal{S}_{\text{eff}}/\hbar} = \left(1 - g_{ib}O_1\left[J_{\mathbf{k}}\right]\right) e^{-\mathcal{S}_{\text{eff}}^F\left[J_{\mathbf{k}}\right]/\hbar} \Big|_{J_{\mathbf{k}}=0},$$
(3.16)

where $O_1[J_{\mathbf{k}}]$ is given by

$$O_{1}[J_{\mathbf{k}}] = \frac{g_{ib}^{2}n_{0}}{\hbar (2\hbar V)^{2}} \sum_{\mathbf{k}_{1},\mathbf{k}_{2}} V_{\mathbf{k}_{1}}^{2} V_{\mathbf{k}_{2}}^{2} \int_{0}^{\hbar\beta} d\tau_{1} \int_{0}^{\hbar\beta} d\tau_{2} \int_{0}^{\hbar\beta} d\tau_{3} \left[\rho_{\mathbf{k}_{1}}^{*}(\tau_{1}) + J_{\mathbf{k}_{1}}^{*}(\tau_{1}) \right] \\ \times \rho_{\mathbf{k}_{1}}(\tau_{2})\rho_{\mathbf{k}_{2}}^{*}(\tau_{2}) \left[\rho_{\mathbf{k}_{2}}(\tau_{3}) + J_{\mathbf{k}_{2}}(\tau_{3}) \right] \mathcal{G}_{\mathbf{k}_{1}}(\tau_{1} - \tau_{2}) \mathcal{G}_{\mathbf{k}_{2}}(\tau_{2} - \tau_{3}). \quad (3.17)$$

This term can be interpreted in relation to a process where an impurity creates an excitation out of the BEC at time τ_1 , scatters with this excitation at time τ_2 , and finally returns it to the BEC at time τ_3 . Hence we will refer to this term as the

first-order scattering term. Every higher order term in the expansion will contain precisely one combination where every pair of functional derivatives is applied only to the exponential and contributes a power of O_1 . A short calculation shows that these terms form the exponential power series:

$$e^{-S_{\rm eff}/\hbar} = \left[\sum_{n=0}^{\infty} \frac{(-1)^n g_{ib}^n O_1^n}{n!}\right] e^{-S_{\rm eff}^F/\hbar}.$$
 (3.18)

Here, we use O_1 as a notation for $O_1[J_{\mathbf{k}}=0]$, i.e. where the source terms are set to zero. We can proceed to derive the second-order scattering term O_2 . The n = 2 term in the expansion of (3.11) can be written as:

$$\frac{1}{2!}\frac{\hbar}{n_0}\sum_{\mathbf{k},\mathbf{s}}\int_0^{\hbar\beta} d\tau \rho_{\mathbf{k}-\mathbf{s}}(\tau) \frac{\delta}{\delta J_{\mathbf{k}}(\tau)} \frac{\delta}{\delta J_{\mathbf{s}}^*(\tau)} O_1\left[J_{\mathbf{k}}\right] e^{-\mathcal{S}_{\text{eff}}^F[J_{\mathbf{k}}]/\hbar} \Big|_{J_{\mathbf{k}}=0}.$$
(3.19)

Applying one of the two functional derivatives in (3.19) to the exponential and the other to $O_1[J_k]$ and vice versa will result in two terms that are combined in:

$$g_{ib}^2 O_2\left[J_{\mathbf{k}}\right] e^{-\mathcal{S}_{\text{eff}}^F\left[J_{\mathbf{k}}\right]/\hbar} \Big|_{J_{\mathbf{k}}=0}, \qquad (3.20)$$

where

$$O_{2}[J_{\mathbf{k}}] = \frac{g_{ib}^{2}n_{0}}{(2\hbar V)^{3}\hbar} \sum_{\mathbf{k_{1},k_{2},k_{3}}} V_{\mathbf{k_{1}}}^{2}V_{\mathbf{k_{2}}}^{2}V_{\mathbf{k_{3}}}^{2} \int_{0}^{\hbar\beta} d\tau_{1} \int_{0}^{\hbar\beta} d\tau_{2} \int_{0}^{\hbar\beta} d\tau_{3} \int_{0}^{\hbar\beta} d\tau_{4} \\ \times \left[\rho_{\mathbf{k_{1}}}^{*}(\tau_{1}) + J_{\mathbf{k_{1}}}^{*}(\tau_{1})\right] \rho_{\mathbf{k_{1}}}(\tau_{2})\rho_{\mathbf{k_{2}}}^{*}(\tau_{2})\rho_{\mathbf{k_{2}}}(\tau_{3})\rho_{\mathbf{k_{3}}}^{*}(\tau_{3}) \left[\rho_{\mathbf{k_{3}}}(\tau_{4}) + J_{\mathbf{k_{3}}}(\tau_{4})\right] \\ \times \mathcal{G}_{\mathbf{k_{1}}}(\tau_{1} - \tau_{2}) \mathcal{G}_{\mathbf{k_{2}}}(\tau_{2} - \tau_{3}) \mathcal{G}_{\mathbf{k_{3}}}(\tau_{3} - \tau_{4}).$$
(3.21)

For every term of order n > 2 in the expansion there will be a combination of functional derivatives that will result in a contribution $\sim (n)(n-1)O_1^{n-2}O_2$. Performing the explicit calculation shows that these terms can be combined with the series of first-order scattering terms in (3.18) in the following way:

$$e^{-S_{\text{eff}}/\hbar} = \left[\sum_{n=0}^{\infty} \frac{(-1)^n g_{ib}^n O_1^n}{n!}\right] \left(1 + g_{ib}^2 O_2\right) e^{-S_{\text{eff}}^F/\hbar}.$$
 (3.22)

We will return to the factorization pattern appearing in (3.22) later. First we have to address the terms that are not included in this reasoning.

3.2.3 Excitation bath terms

In the n = 2 order of the expansion we could have also chosen to apply both functional derivatives to $O_1[J_k]$ in expression (3.19), which would result in:

$$g_{ib}^2 \frac{\tilde{O}_1}{2} e^{-\mathcal{S}_{\text{eff}}^F/\hbar},\tag{3.23}$$

where

$$\tilde{O}_{1} = \frac{1}{(2\hbar V)^{2}} \sum_{\mathbf{k_{1},k_{2}}} V_{\mathbf{k_{1}}}^{2} V_{\mathbf{k_{2}}}^{2} \int_{0}^{\hbar\beta} d\tau_{1} \int_{0}^{\hbar\beta} d\tau_{2} \rho_{\mathbf{k_{1}}}(\tau_{1}) \rho_{\mathbf{k_{2}}}^{*}(\tau_{1}) \rho_{\mathbf{k_{2}}}(\tau_{2}) \rho_{\mathbf{k_{1}}}^{*}(\tau_{2}) \times \mathcal{G}_{\mathbf{k_{1}}}(\tau_{1}-\tau_{2}) \mathcal{G}_{\mathbf{k_{2}}}(\tau_{1}-\tau_{2}) . \quad (3.24)$$

This term can be related to a process where an impurity exchanges momentum with the excitation bath without coupling to the BEC, i.e. without creating an excitation from the condensate or scattering it back to the condensate through the original Fröhlich process. Whereas the scattering terms discussed in the previous subsection, such as (3.17), are proportional to n_0 (the number of atoms in the condensate), the enhancement factor n_0 is absent in the excitation bath terms such as (3.24).

The higher-power contributions of this term will present themselves as $\tilde{O}_1^{n/2}$ in all the even n > 2 expansion terms and together with (3.23) they form an exponential power series as well:

$$e^{-\mathcal{S}_{\text{eff}}/\hbar} = \left[\sum_{n=0}^{\infty} \frac{1}{n!} \left(g_{ib}^2 \frac{\tilde{O}_1}{2}\right)^n\right] e^{-S_{\text{eff}}^F/\hbar}.$$
(3.25)

Just like for the scattering terms, this reasoning can be extended to higher order terms \tilde{O}_n or to the combination of these terms with the scattering terms such as $\tilde{O}_1 O_1^{n-2}$. In general, terms uncoupled from the condensate, arise when both functional derivatives $\frac{\delta}{\delta J_{\mathbf{k}}(\tau)} \frac{\delta}{\delta J_{\mathbf{s}}^*(\tau)}$ in a pair in (3.11) are applied to the two source terms contained in a scattering term $O_n [J_{\mathbf{k}}]$. As mentioned above, the main difference between the scattering terms and the excitation bath terms is that the former contain a leading order n_0 , while the latter do not and are therefore suppressed by a relative factor of a_{bb}/ξ , with a_{bb} the boson-boson scattering length and ξ the coherence length of the BEC. Within the range of validity of the Bogoliubov approximation, i.e. $(n_0 a_{bb}^3) \ll 1$, they are negligible. Note that a similar argument has been made in a perturbative calculation [92] to ignore diagrams where the impurity couples to bosons outside of the BEC. We will therefore not include these excitation bath terms in the rest of our calculations.

Note that in a more recent study of a similar path integral problem for the anharmonic solid state polaron [91] an additional factor 1/2 is obtained in front of the \tilde{O}_1 term (3.24), which is indicative of overcounting terms in our argument. Taking a closer look and comparing with [91], we can see that by following Feynman's argument [62], which was valid for the Fröhlich model, and integrating over all possible $\{Q_{\mathbf{k}}, Q_{\mathbf{k}}^*\}$ as we have done here, we do indeed make the error of counting each \tilde{O}_n twice for each $Q_{\mathbf{k}}^* = Q_{-\mathbf{k}}$. This subtlety was missed in our original study [81] since the \tilde{O}_n terms were dropped from this point onwards. Fortunately, this counting problem is not present for the O_n terms which are in exact agreement with [91] as their origin is different. In summary, aside from this small inconsequential error, our approach in this chapter remains valid.

3.2.4 Result

In the discussion of the scattering terms above we have found that the power series in the first-order terms O_1 and all the product terms $O_2O_1^{n-2}$ compactly factorize in expression (3.22). An explicit calculation shows that this factorization pattern extends to higher-order scattering terms O_n :

$$e^{-\mathcal{S}_{\text{eff}}/\hbar} = \left(\sum_{n=0}^{\infty} \frac{(-1)^n g_{ib}^n}{n!} O_1^n\right) \times \left(1 + g_{ib}^2 O_2 + \frac{g_{ib}^4}{2!} O_2^2 + ...\right) \\ \times \left(1 - g_{ib}^3 O_3 + ...\right) \times (...) e^{-\mathcal{S}_{\text{eff}}^F/\hbar}.$$
(3.26)

Here, O_n represents an *n*-th order scattering process where an impurity creates an excitation out of the BEC and scatters with it *n* times before scattering it into the condensate again:

$$O_{n} = \frac{g_{ib}^{2} n_{0}}{\hbar \left(2V\hbar\right)^{n+1}} \int_{0}^{\hbar\beta} d\tau_{1} \dots \int_{0}^{\hbar\beta} d\tau_{n+2} \\ \times \sum_{\mathbf{k}_{1},\dots,\mathbf{k}_{n+1}} \left(\prod_{j=1}^{n+1} V_{\mathbf{k}_{j}}^{2} \mathcal{G}_{\mathbf{k}_{j}} \left(\tau_{j+1} - \tau_{j}\right) \rho_{\mathbf{k}_{j}}(\tau_{j})^{*} \rho_{\mathbf{k}_{j}}(\tau_{j+1})\right).$$
(3.27)

The factorization pattern appearing in (3.26) suggests that the effective action can be written as:

$$\mathcal{S}_{\text{eff}} = \mathcal{S}_{\text{eff}}^F - \hbar \sum_{n=1}^{\infty} (-1)^n g_{ib}^n O_n.$$
(3.28)

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As we have mentioned before, the more recent approach to these types of path integrals [91] yields exactly the same O_n terms and confirms validity of the effective action (3.28) that will be used from this point onwards. It might be illustrative to point out that even within the conventional Fröhlich model a similar structure can be observed. Performing a perturbative expansion of the Fröhlich contribution in (3.7) with respect to the free impurity yields:

$$e^{-S_{\text{eff}}^F/\hbar} = \left(1 + O_0 + \frac{1}{2!}O_0^2 + ...\right)e^{-S_{\text{free}}/\hbar},$$
 (3.29)

where S_{free} is the action functional of a non-interacting impurity and O_0 is a "zeroth-order" scattering term characterizing an impurity that creates an excitation and absorbs it a time later, without any interaction in between. This series can be resummed to obtain precisely the effective action of the Fröhlich model (3.10).

In what follows we will study the extended action, once again relying on the Jensen-Feynman inequality:

$$F \le F_0 + \frac{1}{\hbar\beta} \left\langle \mathcal{S}_{\text{eff}} - \mathcal{S}_0 \right\rangle.$$
(3.30)

In contrast to the previous chapter, here we will use the simpler Feynman model action with two variational parameters M and W:

$$S_0 = \int_0^{\hbar\beta} \frac{m\dot{\mathbf{r}}^2}{2} dt + \frac{MW^3}{8} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma \frac{\cosh\left[W\left(u - \hbar\beta/2\right)\right]}{\sinh\left(W\hbar\beta/2\right)} \left[\mathbf{r}(\tau) - \mathbf{r}(\sigma)\right]^2.$$
(3.31)

The reason for this is twofold. First, the studies in this thesis have chronologically not been performed in the same order as the chapters. At the moment of this study we have not yet been employing the general memory kernel approach discussed in Chapter 2. Second, as we will see, the simpler variational method will already be sufficient to understand the ground state properties of the system and provide good agreement with other approaches to the extended Hamiltonian. The difficulty in applying the inequality to the extended model is that the expectation value of the effective action (3.28) contains impurity density correlation functions at different times, of an arbitrarily large order corresponding to the number of scattering events in the scattering terms. This can explicitly be seen from the product in (3.27). Unfortunately, we are not aware of any technique to exactly compute such expectation values up to arbitrary order and in the next subsection an approximation will be explored.

3.2.5 RANDOM PHASE APPROXIMATION

To proceed analytically, an approximation of the impurity density correlations can be made. Relative to the model system S_0 , the impurity density correlation between the creation of an excitation at time τ_j and its absorption at time τ_{j+1} depends only on the absolute value of the time step [48]:

$$\left\langle \rho_{\mathbf{k}_{j}}^{*}(\tau_{j})\rho_{\mathbf{k}_{j}}(\tau_{j+1})\right\rangle_{0} = \mathcal{F}_{\mathbf{k}_{j}}\left(\left|\tau_{j}-\tau_{j+1}\right|\right).$$
(3.32)

For Feynman's model action the memory function of the impurity $\mathcal{F}_{\mathbf{k}}(u)$ is given by:

$$\mathcal{F}_{\mathbf{k}}(u) = \exp\left(\frac{\hbar k^2}{2\left(M+m\right)} \left[\frac{u^2}{\hbar\beta} - u + \frac{M}{\Omega m} \frac{\cosh\left(\Omega\left[\hbar\beta/2 - u\right]\right) - \cosh\left(\hbar\beta\Omega/2\right)}{\sinh\left(\hbar\beta\Omega/2\right)}\right]\right).$$
(3.33)

We consider a random phase approximation (RPA) where the dominant contribution to the correlation of a number of subsequent scattering events is given by the correlations within one scattering event (3.32):

$$\left\langle \prod_{j=1}^{n+1} \rho_{\mathbf{k}_{j}}^{*}(\tau_{j}) \rho_{\mathbf{k}_{j}}(t_{j+1}) \right\rangle_{0} \approx \prod_{j=1}^{n+1} \left\langle \rho_{\mathbf{k}_{j}}^{*}(\tau_{j}) \rho_{\mathbf{k}_{j}}(\tau_{j+1}) \right\rangle_{0} = \prod_{j=1}^{n+1} \mathcal{F}_{\mathbf{k}_{j}}\left(|\tau_{j} - \tau_{j+1}| \right).$$
(3.34)

Using $\mathcal{G}_{\mathbf{k}_{j}}(\hbar\beta - u) = \mathcal{G}_{\mathbf{k}_{j}}(u)$ and $\mathcal{F}_{\mathbf{k}_{j}}(\hbar\beta - u) = \mathcal{F}_{\mathbf{k}_{j}}(u)$ it is not difficult to show that within this approximation the additional contributions to the effective action constitute a power series:

$$\left\langle \mathcal{S}_{\text{eff}} \right\rangle_{0} = \left\langle \mathcal{S}_{\text{eff}}^{F} \right\rangle_{0} + g_{ib} n_{0} \hbar \beta \sum_{n=2}^{\infty} \left(-\frac{g_{ib}}{\hbar V} \sum_{\mathbf{k}} V_{\mathbf{k}}^{2} \int_{0}^{\hbar \beta/2} du \mathcal{G}_{\mathbf{k}}\left(u\right) \mathcal{F}_{\mathbf{k}}\left(u\right) \right)^{n}.$$
 (3.35)

After substituting the expectation value of the Fröhlich effective action (3.7) with respect to the variational model system and adding the first-order energy contribution $g_{ib}n_0$, the expectation value of the full effective action becomes:

$$\left\langle \mathcal{S}_{\text{eff}} \right\rangle_{0} = \left\langle \int_{0}^{\hbar\beta} \frac{m\dot{\mathbf{r}}^{2}}{2} \right\rangle_{0} + g_{ib}n_{0}\hbar\beta \sum_{n=0}^{\infty} \left(-\frac{g_{ib}}{\hbar V} \sum_{\mathbf{k}} V_{\mathbf{k}}^{2} \int_{0}^{\hbar\beta/2} du \mathcal{G}_{\mathbf{k}}\left(u\right) \mathcal{F}_{\mathbf{k}}\left(u\right) \right)^{n}.$$
(3.36)

Each term inside the round brackets in (3.36) exhibits a UV divergence linear in the UV cutoff Λ in the momentum integral. Therefore, the full effective action

contains an entire polynomial series of divergences:

$$\langle \mathcal{S}_{\text{eff}} \rangle_{0}^{(\text{UV})} \sim \sum_{n} g_{ib}^{n+1} \mathcal{O}\left(\Lambda^{n}\right).$$
 (3.37)

In contrast to the case for the Bogoliubov-Fröhlich model discussed in Chapter 1 where a second order correction in (1.43) was sufficient, this series can only be exactly regularized by substituting the *full* Lippmann-Schwinger equation:

$$g_{ib}^{-1} = \frac{\mu}{2\pi\hbar^2 a_{ib}} - \frac{1}{V} \sum_{\mathbf{k}} \frac{2\mu}{\hbar^2 k^2},$$
(3.38)

where $\mu = \left(m_b^{-1} + m^{-1}\right)^{-1}$ is the reduced impurity-boson mass and a_{ib} is the impurity-boson scattering length. The free energy F_0 of the model system and expectation value of the action of the model system $\langle S_0 \rangle_0$ can be computed. Substitution into the Jensen-Feynman inequality (3.30) yields the following variational free energy:

$$F = \frac{3}{\beta} \ln \left[\sinh \left(\frac{\hbar \beta \Omega}{2} \right) \right] - \frac{3}{\beta} \ln \left[\sinh \left(\frac{\hbar \beta W}{2} \right) \right] - \frac{3}{2\beta} \ln \left(\frac{m+M}{m} \right) - \frac{3}{2\beta} \frac{M}{M+m} \left[\frac{\hbar \beta \Omega}{2} \coth \left(\frac{\hbar \beta \Omega}{2} \right) - 1 \right] + \frac{2\pi \hbar^2 n_0}{\mu} \frac{1}{a_{ib}^{-1} - a_0^{-1}(M,\Omega,\beta)}.$$
(3.39)

Strictly speaking, by making the approximation in this section the variational inequality is no longer guaranteed. However, unless divergences are found, on the premise that the approximation makes a small error we proceed to use (3.39) as an approximate variational expression. The variational parameters are Ω and M and the relation between Ω and the original oscillator frequency in the model system is given by $\Omega = W\sqrt{1 + M/m}$, see [8, 48, 62] for a detailed description. The free energy (3.39) is written in a suggestive form to make the analogy with the resonance shift observed in [50, 70]. The resonance shift is UV convergent and in our case depends on both the temperature and the variational parameters:

$$a_0^{-1}(M,\Omega,\beta) = \frac{2\pi\hbar^2}{\mu V} \left[\sum_{\mathbf{k}} \frac{2\mu}{\hbar^2 k^2} - \frac{1}{\hbar} \sum_{\mathbf{k}} V_{\mathbf{k}}^2 \int_0^{\hbar\beta/2} du \mathcal{G}_{\mathbf{k}}\left(u\right) \mathcal{F}_{\mathbf{k}}\left(u\right) \right].$$
(3.40)

Note that to be able to neatly write the energy in this way, we have explicitly added the mean field energy contribution $2\pi\hbar^2 a_{ib}n_0/\mu$ to the energy, which is not included in the expression given in [48]. Therefore the *polaronic* energy contribution is given by $F - g_{ib}n_0$ with F as the optimal variational energy.

As a consistency check we consider the limit of weak coupling with a simplified model system where the phonon mass of the Feynman model approaches zero, $M \to 0$, while the spring constant MW^2 remains fixed. At zero temperature $(\beta \to \infty)$, the energy in the weak coupling limit E_{weak} is independent of the variational parameters and given by:

$$E_{\text{weak}} = \frac{2\pi\hbar^2 n_0}{\mu} \frac{1}{a_{ib}^{-1} - a_{0,\text{weak}}^{-1}}.$$
(3.41)

In this limit the *u*-integral in $a_{0,\text{weak}}^{-1}$ can be analytically performed:

$$a_{0,\text{weak}}^{-1} = \frac{2\pi\hbar^2}{\mu V} \left[\sum_{\mathbf{k}} \frac{2\mu}{\hbar^2 k^2} - \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^2}{\hbar\omega_{\mathbf{k}} + \frac{\hbar^2 k^2}{2m}} \right].$$
 (3.42)

Expression (3.41) with the resonance shift (3.42) is precisely the mean-field result including extended interactions at zero polaron momentum $\mathbf{P} = 0$ [50, 59], which provides a confirmation of our result.

Feynman's path-integral formalism allows us to calculate an effective mass for the polaron m_{pol} and a root mean square (RMS) estimate of the polaron size $\sqrt{\langle \mathbf{r}^2 \rangle}$. The expression for the polaron radius depends only on the model system and remains the same as in [48]:

$$\left\langle r^2 \right\rangle = \frac{3\hbar}{2\Omega} \frac{m+M}{mM} \coth\left(\frac{\hbar\beta\Omega}{2}\right).$$
 (3.43)

In Chapter 2 we have already discussed obtaining the polaron effective mass by introducing a boost to the memory function of the system $\langle \exp(i\mathbf{k} [\mathbf{r}(\tau) - \mathbf{r}(\sigma)]) \rangle_0 \rightarrow \langle \exp(i\mathbf{k} [\mathbf{r}(\tau) - \mathbf{r}(\sigma)]) \rangle_0 \times \exp(i\mathbf{k} \cdot \mathbf{v}(\tau - \sigma))$. This method is used in Feynman's seminal work on polarons within the Fröhlich model [8, 62]. However, to incorporate the effects on the effective mass of the extended Fröhlich contributions we only apply this boost to the effective action after the RPA contributions have been separated in (3.36). After deriving the energy as a function of \mathbf{v} and expanding it up to \mathbf{v}^2 , the factor in front of $\mathbf{v}^2/2$ can be identified as the polaron effective mass:

$$m_{\rm pol} = m + \lim_{\beta \to \infty} \frac{4}{3} \frac{\pi^2 \hbar^3 n_0}{\mu^2} \frac{\Gamma(M, \Omega, \beta)}{\left(a_{ib}^{-1} - a_0^{-1}(M, \Omega, \beta)\right)^2},\tag{3.44}$$

where Γ is given by:

$$\Gamma(M,\Omega,\beta) = \frac{1}{V} \sum_{\mathbf{k}} k^2 V_{\mathbf{k}}^2 \int_0^\infty du \, u^2 \mathcal{G}_{\mathbf{k}}(u) \,\mathcal{F}_{\mathbf{k}}(u) \,. \tag{3.45}$$

As far as we are aware, Feynman's prescription is only valid in the low temperature limit, so the limit $\beta \to \infty$ in expression (3.44) must be taken. The effect of temperature is then estimated through the implicit temperature dependence of the variational parameters M and Ω , as has been done in [86]. Note that in the limit of $M \to 0$ in the model system, also our result for the effective mass reduces to the extended Fröhlich interactions mean-field result [59].

3.3 Results

3.3.1 Comparison with the Fröhlich model for the repulsive polaron

First, we make a direct comparison between the results obtained with Feynman's variational description within the Fröhlich model in [48] and the results including extended interactions derived in the previous section. Because the polaronic contribution to the free energy within the Fröhlich model is the same on both sides of the resonance we will only consider the repulsive polaron in this section. It is important to note that on this side of the resonance various shallow bound states are expected to exist at lower energies [49, 50] and we are only retrieving the energy of the repulsive branch in our approach. We do not observe direct evidence of Efimov bound states for an impurity in a BEC [42–44] in this approach, but we keep open to the possibility that their effect on the repulsive branch is captured. Within the Fröhlich model, the results at a given temperature can be expressed as a function of a single dimensionless polaronic coupling constant $\alpha = a_{ib}^2/(\xi a_{bb})$. However, for (3.39) this is no longer the case, as the results depend also explicitly on a_{bb} and hence in the extended model the coupling constant α is no longer particularly useful. Nevertheless, for a fixed a_{bb} we can still plot our results as a function of α at the repulsive side of the resonance for the purpose of the comparison. Note that while previously we have compared energies at different momentum cutoff values for the purpose of benchmarking different theoretical approaches, in real systems a finite physical cutoff scale can be identified. In atomic gases the natural cutoff corresponds to the range of the interatomic interaction,

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FIGURE 3.1: A comparison of the polaronic contribution to the free energy including extended interactions (dashed lines) with that of the Fröhlich model (full lines) as a function of the coupling constant α at various temperatures $\beta = \hbar^2/(mk_BT\xi^2) = [4, 8, 20, 100]$. For the purpose of the comparison with [48], the same impurity-condensate parameters are taken: $m_b = 3.8 m$, $\xi = 450 nm$, and $a_{bb} = 2.8 nm$. The inset shows the same results at stronger coupling.



FIGURE 3.2: A comparison of the RMS polaron radius of Feynman's approach including extended interactions (dashed lines) with that of the Fröhlich model (full lines) as a function of the coupling constant α at various temperatures. The same impurity-gas parameters are used as in Figure 3.1.

given by $\Lambda_c \approx 200\xi^{-1}$ for the current system which will be used for the comparison.

Figure 3.1 shows the results for the polaronic contribution to the free energy $F_p = F - 2\pi\hbar^2 a_{ib}n_0/\mu$, in polaronic units ($\xi = m = \hbar = 1$) at various temperatures. At weak coupling both results coincide but they start to significantly differ around $\alpha \approx 3.5$ where the Fröhlich model predicts a very steep decrease in energy, indicative of self-trapping. The extended interactions appear to moderate this into a much slower linear decrease of the free energy. The decrease of the polaronic contribution is even slower than the increase of the first-order contribution $2\pi\hbar^2 a_{ib}n_0/\mu$, and the full polaron energy for the extended interactions model never becomes negative.

Figure 3.2 presents a comparison of the polaron RMS radius (3.43) between the two models. The first noticeable difference is that the sharp kink within the Fröhlich model, previously identified with the transition into the strong coupling regime around $\alpha = 3.5$, is replaced by a smoother non-monotonic transition due to the extended interactions. Most significant is the difference at extremely strong coupling however. The inclusion of the extended interactions disproves previous predictions of the asymptotically shrinking Bose polaron within this method, which was suggestive of self-trapping as well, and shows that the polaron radius approaches a finite non-zero value around $\approx 0.35\xi$. Comparable conclusions follow for the effective mass of the polaron (3.44), shown in Figure 3.3. The effective

3.3 - Results



FIGURE 3.3: A comparison of the polaron effective mass of Feynman's approach including extended interactions (dashed lines) with that of the Fröhlich model (full lines) as a function of the coupling constant α at various temperatures. The same impurity-gas parameters are used as in Figure 3.1.

mass no longer exhibits a sudden and steep transition into the strong coupling regime. A period of faster increase of the effective mass is still observed around $\alpha = 5$ -10, but flattens out towards a value of roughly $\approx 20m$ at even stronger coupling. Furthermore we can see that in the case of a light impurity such as considered here, the effective mass is more sensitive to temperature differences than the energy and radius. It has been pointed out that measurements of the effective mass of the polaron are expected to be particularly useful to discern between various theoretical models [57, 68]. Based on our results we expect this to be even more the case when the temperature dependence is measured as well.

The converging effective mass and polaron radius together with the positive free energy suggest that self-trapping does not take place for the repulsive polaron when the extended interactions are included. This is qualitatively in agreement with the findings of the RG approach [70], where no self-trapping is observed for the repulsive polaron.

3.3.2 Comparison with other theoretical results

In this subsection we provide a comparison with other recent results in the literature, specifically with the mean-field approach [50], the RG approach [68] and Quantum Monte Carlo (QMC) calculations [46]. As mentioned above, the mean-

field expressions for the energy and effective mass [50, 59] can also be obtained from the weak coupling limit of Feynman's model.

Before proceeding to the discussion, one aspect of the Feynman model has to be addressed. As can be seen from expression (3.39), the variational landscape can contain poles where the free energy diverges to negative (or positive) infinity, accompanied by a divergence of the effective mass (3.44). On the negative side of the resonance, even at weaker coupling, these poles are present. However, below a critical coupling strength there exists a separated local minimum that corresponds to the polaronic state. To plot the polaron energy of the attractive branch we follow this local minimum starting from weak interactions up to the point where it merges with one of the aforementioned poles, at which both the energy and effective mass diverge.

To better understand the physical significance of these divergences, it is illustrative to observe that the same type of pole is present in the extended mean-field treatment [50, 59], where it is independent of any additional variational parameters. In the MF model this divergence can be shown to be accompanied by a rapid depletion of the BEC, which is no longer accurately described within Bogoliubov theory. We therefore believe that the poles observed within our treatment can be interpreted as a runaway pathway related to the shortcomings of the Bogoliubov approximation and regardless of the underlying physical reason for the divergence the inclusion of higher order boson interactions should have a stabilizing effect. A detailed discussion of similar divergences, observed in RG theory, is presented in [70]. Note that in [44] no divergences are observed for the polaron at unitarity, which we have initially interpreted as a stabilizing effect from Efimov physics. However in approaches in lines of [44] only a small number of phonon excitations are allowed and hence divergences associated with an infinite number of phonons cannot be found. In a more recent study of the extended Fröhlich model [45] within an approach that has been shown to capture Efimov physics and in addition allows for an infinite number of excitations, qualitatively similar behavior to our results is observed where a metastable state transitions into an unstable state on the attractive branch due to the effect of Efimov physics. Therefore in retrospect this provides indication that our approach and RG might be capturing traces of Efimov physics.

For the repulsive polaron no runaway pathways exist at weak coupling and we simply follow the global minimum of the variational landscape. Only at extremely strong coupling, separated divergences start to appear and the polaronic

3.3 - Results



FIGURE 3.4: A comparison of the polaron energy obtained with the path-integral variational method including extended interactions (solid), the mean-field model including extended interactions [50] (dotted), the RG approach [70] (connected dots) and QMC [46] (diamonds). The impurity and condensate parameters correspond to the experiment of Jørgensen et al. [23], given by $m = m_b$ and $a_{bb} = 9a_0$, a_0 being the Bohr radius. We take a UV momentum cutoff of the range of the Feshbach resonance $\Lambda_c = (60a_0)^{-1} \approx 190\xi^{-1}$ in this experiment, given in [23] and also used in [70]. On the figure the inverse scattering length is measured in terms of $k_n = (6\pi^2 n_0)^{1/3}$. The temperature integral cutoff corresponds to $\beta_c = \hbar^2/(\xi^2 m k_B T) = 200$ or 0.17 nK. For the purpose of the comparison with RG we plot the repulsive branch up to $(k_n a_{ib})^{-1} \approx 0.18$. On the attractive branch we can only show the RG data up to the lower range of fig. 9 in [70]. The inset shows the high cutoff behavior of $E(\Lambda)/E(\Lambda_c)$ in the Feynman approach at strong coupling for $(k_n a_{ib})^{-1} = 0.3$.

state becomes a local minimum. This local minimum continues to exist across the resonance towards negative scattering lengths, and it is not clear if we can interpret it as the repulsive polaron state from this point on. For the purpose of the comparison with RG in this subsection, we will restrict our study of the repulsive branch to couplings below the critical coupling presented in [70]. At this point the aforementioned transition into a local minimum has not yet taken place.

Figures 3.4 and 3.5 show a comparison of the polaron energies obtained with various methods, across the resonance for impurity-condensate parameters used in the experiments [23] and [19], respectively. To provide an accurate comparison with RG, the same respective finite values of the momentum cutoff were used as in [70]. As shown on the inset of 3.4, this result is not yet completely converged as a function of the cutoff which is here taken to correspond to the physical length scales associated with the interatomic potential. As we have discussed in great detail in Chapter 2, the Bose polaron models are not necessarily UV convergent in the $\Lambda \rightarrow \infty$ case when more advanced methods are used. For the purpose of the comparison in Figure 3.4, where a relatively small cutoff is used, we do not expect the logarithmic divergence to be of great importance. For both calculations finite temperatures, at which the energy has converged beyond any noticeable difference in the figures, were used to represent zero temperature. This convergence is shown on the inset of 3.5.

For the repulsive polaron we observe a relatively good quantitative agreement with QMC data in Figure 3.4 and an excellent agreement in Figure 3.5. Note, however, that the QMC calculation does not rely on the Bogoliubov approximation and hence the comparison is made within different models of the Bose polaron. Our results predict no divergence of the repulsive branch energy in contrast to the mean-field treatment, but towards stronger coupling a quantitative discrepancy with the RG approach appears. However, as shown in Figure 3.6, a much better agreement exists for the effective mass of the repulsive polaron between the two methods. One possible explanation for the discrepancy in energy is the previously discussed logarithmic divergence captured in the RG theory, to capture which we need our more advanced approach of Chapter 2. The QMC study [46] does not elaborate on the cutoff dependence so the status of the logarithmic divergences in this method is unclear. On the negative side of the resonance we see qualitative agreement with RG where the polaron energy and effective mass diverge at a weaker interaction strength than predicted by the mean-field description or QMC.

The theoretical results can also be compared to the experimental data points

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FIGURE 3.5: A comparison of the polaron energy obtained with the path-integral variational method including extended interactions (solid), the mean-field model including extended interactions [50] (dotted), the RG approach [70] (connected dots) and QMC [46] (diamonds). The impurity and condensate parameters correspond to the experiment of Hu et al. [19], given by $m_b = 2.17m$ and $a_{bb} = 100a_0$, a_0 being the Bohr radius. We take the same UV cutoff $\Lambda_c = 10^3/\xi$ as used in [70]. The temperature integral cutoff corresponds to $\beta_c = \hbar^2/(\xi^2 m k_B T) = 1000$ or 0.3 nK. For the purpose of the comparison with RG we plot the repulsive branch up to $(k_n a_{ib})^{-1} \approx 0.25$. The inset shows the low temperature convergence of $E(\beta)/E(\beta_c)$ in the Feynman approach at strong coupling for $(k_n a_{ib})^{-1} = 0.3$.



FIGURE 3.6: A comparison of the polaron effective mass between Feynman's model including extended interactions (solid), the mean-field model including extended interactions [50, 59] (dotted) and the RG approach [70] (connected dots). The same impurity-condensate parameters were used as in 3.4 corresponding to the experiment of Jørgensen et al. [23]. For the purpose of the comparison with RG we plot the repulsive branch up to $(k_n a_{ib})^{-1} \approx 0.18$.

from [19, 23], which we have not explicitly added to the figures for the purpose of clarity. At weak coupling all theoretical approaches are in excellent agreement with experiments. For the repulsive branch as the coupling gets stronger, the data points of Jørgensen et al. [23] lie at higher energies than QMC, even after the non-homogeneity of the three-body decay processes is taken into account in the spectroscopic signal [46]. As both RG and our results lie below QMC it follows that the agreement with this experiment is not close in this regime. Several reasons for this discrepancy are suggested in [46]. In contrast we find excellent agreement with the experiment of Hu et al. [19] on the repulsive branch, which is also in much closer agreement with QMC than the Jørgensen et al. experiment. The early divergence for the attractive polaron that is found in our results and the RG approach is observed in neither experiment, and as mentioned above, its understanding requires a further study of the validity of the Bogoliubov approximation and the effects of Efimov physics in that regime.



FIGURE 3.7: The polaronic energy as a function of the interaction ratio $\eta = g_{ib}/g_{bb}$ of Feynman's extended approach is compared to RG theory (connected dots) [94], diffusive Monte Carlo (DMC) calculations (diamonds) [94], the beyond-Fröhlich mean-field approach [50] at zero polaron momentum (to which our theory reduces at weak coupling) and the Feynman-Fröhlich approach [48].

3.4 Results in 1D

The Bose polaron has also been experimentally created in one-dimensional systems by Catani *et al.* [93] in arrays of tubes that contain ≈ 180 bosonic Rb atoms with ≈ 1.4 K impurities per tube. The atoms are strongly trapped in the transverse direction ensuring the 1D regime, and in addition trapped in along the tube direction to stabilize the condensate. The impurities are then localized at the center of the tube with a species-selective dipole beam, after which they are released and imaged afterwards to measure the axial width displacement and the effective (polaron) mass of the impurity.

While a number of open questions surrounding the 3D Bose polaron and the importance of various contributions to the Hamiltonian remain, the 1D Bose polaron is better understood in this regard. In particular, two recent seminal theoretical studies of the problem rely on the RG and Monte Carlo approaches [94] or condensate deformation methods [95] present a thorough discussion of the problem. As argued in [94], the Bogoliubov-Fröhlich Hamiltonian (1.21) and extended Fröhlich Hamiltonian (3.1) can be derived in exactly the same form as they are in 3D, of course given that the operators and integrals are demoted

to 1D. In doing so, a couple of important changes occur. First of all in the $\Lambda \to \infty$ limit, Lippmann-Schwinger regularization is not necessary in 1D and the simple expressions $g_{ib} = -1/(\mu a_{ib})$ and $g_{bb} = -2/(m_b a_{bb})$ yield the scattering lengths. In addition, aside from the polynomial UV divergence it appears that the logarithmic divergence discussed in Chapter 2 is absent in 1D as well. Therefore both the Bogoliubov-Fröhlich model and its extension are well behaved in the UV limit and the difficult problem of capturing phonon entanglement across a broad range of momentum scales is not featured in this system. However, a new *infrared* divergence arises in the $\sim g_{ib} \sum_{\mathbf{k}} v_{\mathbf{k}}^2$ correction to the impurity-condensate mean field energy as derived in (1.26), essentially reflecting the fact that the 1D homogeneous condensate cannot exist. As shown in a comparison between MF and RG in [94], an ad hoc removal of this term corresponds well with a more formal regularization, and hence we simply remove the divergent term from the Hamiltonian. Perhaps the most important feature of the 1D Bose polaron demonstrated in both studies, is the observation that corrections beyond the Bogoliubov approximation containing phonon interactions of third and fourth orders can clearly not be neglected at stronger coupling. For the Bose polaron in 3D the effect of such interactions is not yet completely understood, in particular since the QMC results in Figure 3.4 lie closer to the mean field approach than to more advanced theoretical approaches. To gauge the accuracy of our approach, in what follows we compare the results of Feynman's method as described in this chapter to [94] for the extended Fröhlich Hamiltonian in 1D.

Taking into account the aforementioned modifications into our derivation, the variational energy in 1D at the level of (3.39) is given by:

$$F(M,\Omega) = \frac{1}{\beta} \left[\log \left(2\sinh\left(\hbar\beta\Omega/2\right) \right) - \log\left(2\sinh\left(\hbar\beta W/2\right) \right) \right] - \frac{1}{2\beta} \log\left(\frac{m+M}{m}\right) - \frac{1}{2\beta} \frac{M}{M+m} \left[\frac{\hbar\beta\Omega}{2} \coth\left(\frac{\hbar\beta\Omega}{2}\right) - 1 \right] + \frac{g_{ib}n_0}{1 + \frac{g_{ib}}{\hbar}\Gamma},$$
(3.46)

where:

$$\Gamma = \frac{1}{(2\pi)} \int_0^{\hbar\beta/2} du \int_0^{\Lambda} dk V_k^2 \mathcal{G}_k(u) \mathcal{F}(k, u) .$$
(3.47)

Expression (3.46) is derived on the condition that $g_{ib}\Gamma/\hbar < 1$, but as we will see provides an excellent description if the analytic continuation of the series corresponding to the last term of (3.46) is used. Similarly, the following expression



FIGURE 3.8: The polaronic energy as a function of the interaction ratio $\eta = g_{ib}/g_{bb}$ of Feynman's extended approach is compared to RG theory (connected dots) [94], diffusive Monte Carlo (DMC) calculations (diamonds) [94], the beyond-Fröhlich mean-field approach [50] at zero polaron momentum (to which our theory reduces at weak coupling) and the Feynman-Fröhlich approach [48]. The parameters here are the same as in Figure 3.7, except that a weak boson-boson interaction corresponding to $\gamma = 0.014$ was used.



FIGURE 3.9: The 1D polaron effective mass as a function of the interaction ratio $\eta = g_{ib}/g_{bb}$ of Feynman's extended approach is compared to RG theory (connected dots) [94], diffusive Monte Carlo (DMC) calculations (diamonds) [94], the beyond-Fröhlich mean-field approach [50] at zero polaron momentum (to which our theory reduces at weak coupling) and the Feynman-Fröhlich approach [48].

for the effective mass can be derived in 1D:

$$m_{\rm pol} = m + \frac{g_{ib}^2 n_0}{\hbar} \frac{\tilde{\Gamma}}{\left(1 + \frac{g_{ib}}{\hbar}\Gamma\right)^2},\tag{3.48}$$

where:

$$\tilde{\Gamma} = \frac{1}{(2\pi)} \int_0^{\hbar\beta/2} du \int_0^{\Lambda} dk V_k^2 \mathcal{G}_k(u) \mathcal{F}(k, u) k^2 u^2.$$
(3.49)

First, we can compare our results to the previously discussed article using the RG approach and comparing to diffusive Monte Carlo (DMC) calculations [94] in units of the 2011 Florence group experiment by Catani *et al.* [93]. The boson density is given by $n_0\xi = 1.05$ with $\xi = \hbar/\sqrt{2m_bg_{bb}n_0}$ and the mass ratio corresponds to $m_b/m = 87/41$. From this we can derive g_{bb} and all the parameters besides a_{ib} are fixed. Figure 3.7 presents a comparison of the polaron energy between various approaches as a function of $\eta = g_{ib}/g_{bb}$ up to strong coupling. The RG and DMC data was obtained from [94]. The zero-momentum extended mean-field approach [50] was reproduced by setting M = 0 in our calculations, which corresponds to the method of Shchadilova *et al.* in [50]. We have used the numerical momentum cutoff $\Lambda = 10^3 \xi^{-1}$ and a temperature cutoff



FIGURE 3.10: The polaron energy of Feynman's extended approach is compared to QMC calculations (diamonds) [96] and the Feynman-Fröhlich approach [48] at $\gamma = 0.02$ and $\gamma = 0.2$.

of $\beta = 500$. If the effective interactions between the bosons g_{bb} are decreased by tuning $\gamma = g_{bb}m_b/(\hbar^2 n_0) = 0.014$ for the same system, then the results in Figure 3.8 are found where we still see relatively good agreement with RG, with small differences appearing at strong coupling. This small difference is likely caused by discarding the \tilde{O} -terms in (3.25), for which the argument relies on the three dimensional case. Figures 3.7 and 3.8 also show the diffusive Monte Carlo (DMC) results from [94] applied to the *full* impurity-boson Hamiltonian. This clearly demonstrates how the extended Fröhlich Hamiltonian corrects upon the Bogoliubov-Fröhlich Hamiltonian in the intermediate coupling regime and extends the applicability of the model. While the extended model appears to qualitatively capture the physics correctly, it is clear that for quantitatively exact results at strong coupling further corrections are necessary. For the 1D polaron, this extension has been performed in [95].

We can also make a comparison for the effective mass (3.48) in the Catani *et al.* units in Figure 3.9 and find exact agreement with RG in the strong coupling regime providing another confirmation of the accuracy of our approach. This raises further interest as to why larger differences exist in 3D in Figure 3.6 or Figure 2.6.

Finally, Figure 3.10 presents a comparison between QMC calculations by Parisi *et al.* [96] on the full impurity-boson Hamiltonian and our method for the extended Fröhlich model at $m_b = m$. The authors tune the boson-boson interactions through

the parameter $\gamma = g_{bb}m_b/(\hbar^2 n_0)$ and we compare the two weakest coupling results at $\gamma = 0.02$ and $\gamma = 0.2$ which are expected to be still within the Bogoliubov regime. In [96] the energy is presented on a log-log scale, and since the smallest error in obtaining the data is significant in this case we provide the comparison on a log-log scale as well. On this graph the energy is measured in units of $\epsilon_F = \hbar k_F^2/(2m_b)$ where $k_F = \pi n_0$ and the impurity-boson coupling is quantified by $\tilde{\eta} = 2g_{ib}\mu/(\hbar^2 n_0)$. Once again we can see that in the intermediate coupling regime the extended Fröhlich model is exact, but at stronger coupling quantitative discrepancies appear.

3.5 Conclusion

In this chapter we have studied the ground-state properties of the Bose polaron beyond the Fröhlich paradigm using Feynman's variational path-integral formalism. For this purpose we derived the Lagrangian of an impurity immersed in a condensate within the Bogoliubov approximation. The extended Fröhlich interactions take the form of quadratic position- and velocity-dependent terms in the phonon variables. By expanding the position-dependent terms as a full perturbative series the path integral over the phonon variables can be performed to obtain an effective action. This is done within the Bogoliubov approximation, neglecting perturbative terms that contain no coupling to the condensate. We do not expect the velocitydependent terms to contribute significantly to the ground-state properties based on other theoretical studies in the literature. The Jensen-Feynman inequality provides a variational expression for the upper bound on the free energy. Due to the extended interactions it contains a series of impurity density correlations that, as far as we know, does not reduce to an analytic expression. To proceed analytically a random phase approximation is made that decomposes the higher order impurityexcitation scattering correlations as a product of subsequent scattering correlations. The RPA yields simple variational expressions for the polaron energy and effective mass that reduce to the extended Fröhlich mean-field results in the weak coupling limit. For the repulsive polaron we compared the predictions with those of the Fröhlich model and found that the sharp transition to the strong coupling regime, which was interpreted as a possible shortcoming of the path-integral approach for the Fröhlich model, is now replaced by a smooth crossover suggestive of the absence of self-trapping. For the attractive polaron we observed an abrupt divergence of the energy and effective mass at a certain critical coupling strength. This is related to the local polaronic minimum getting absorbed by a runaway pathway in the variational landscape, and is interpreted as a breakdown of the Bogoliubov approximation within our approach. Application of this method in 1D shows excellent agreement with other theoretical studies of the extended Fröhlich Hamiltonian and provides a justification to the approximations made in the derivation. In conclusion, we present a different approach to a problem that is currently under extensive theoretical and experimental investigation, which provides insight into how different processes arise and contribute to the ground state properties of the system.

Various future perspectives for this method exist. While Feynman's method in theory captures the full effect of the excitations at the level of the effective action, it relies on a simple two-parameter model system to capture their influence on the impurity at the level of the free energy and effective mass. Moreover, we invoked an additional approximation by using the random phase approximation. One future perspective would be to consider an application of the general memory kernel approach developed in Chapter 2 to this extended Fröhlich Hamiltonian as well. Finally, at the impurity densities created in current experiments, many-polaron effects are expected to be non-negligible already on a mean-field level [59]. The variational path-integral approach has been used to study these effects for Fröhlich polarons in solids [97, 98] and was applied to the study of the Bose bipolaron within the Fröhlich model [99]. Combining the inclusion of the extended interactions and the approximations made in this chapter with these methods would open a possible avenue towards the study of bipolarons and many-polaron effects in Bose gases beyond the mean-field level with the path-integral formalism.

$_{\rm CHAPTER} 4$

Path integral techniques for many particles with general memory: Partition function

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So far we have explored the path integral approach for a single impurity immersed in a condensate. In Chapter 2 we have seen that in contrast to the previously studied polaronic systems, even for the compact Bogoliubov-Fröhlich Hamiltonian which approximates the Bose polaron system at weaker coupling, significant extensions to the variational approach are required to exactly capture the ground state energy of the system. In Chapter 3 we have further demonstrated the utility of the variational path integral approach for this problem and shown that it can also be applied to more extended Hamiltonians that correct the simpler Bogoliubov-Fröhlich Hamiltonian. Due to growing interest in the Bose polaron problem, in the recent years various other beyond mean field approaches such as RG or the method of Gaussian variational states have been applied to this problem to which an extensive comparison was made in the previous chapters.

All of the aforementioned approaches, including the one presented in this thesis, have so far been mainly focused on a single impurity. However, in typical CHAPTER 4 - PATH INTEGRAL TECHNIQUES FOR MANY PARTICLES WITH GENERAL MEMORY

experiments the impurities are created at finite numbers. A rough estimation of the distances between the impurities in the experiment of [23] quickly yields scales of comparable order to the condensate coherence length ξ and hence one would naturally expect the polarons to interact with one another. In the Aarhus experiment [23] the surprising observation is made that the energy per polaron is barely dependent on the impurity fraction in the condensate, which indicates that the ground state of a single polaron is not affected by the presence of other impurities. In the JILA experiment [19] such a measurement has not been performed which is the reason why we will more closely focus on the Aarhus system [23] in what follows. The relevance of this observation of course hinges on the fact that the single- or many-polaron ground state has completely been reached in the experimental time window, a question towards which efforts are being made in further experimental investigation.

More recently, the dynamics of polaron formation has been at the heart of two experimental studies [25, 100] which indicate that the attractive single polaron ground state is indeed formed in the typical experimental regimes considered in [23]. However, for the repulsive branch no results are presented and hence no conclusive remarks can be made. In addition, an investigation of the many polaron ground state is not performed in the experiments and its formation remains an open question. Nevertheless, the experimental studies emphasize the interest of future studies at higher impurity densities for the purpose of understanding many-polaron interactions, including the repulsive branch [25, 100]. The theoretical study in the rest of this thesis will be aimed at taking steps towards this direction.

Appreciable efforts have already been performed to theoretically understand the many polaron ground state. Initial studies employing a mean field theory [101] or the path integral approach [99] have studied the many polaron effects at the level of the Bogoliubov-Fröhlich Hamiltonian. However, as we have argued before, even for a singly impurity in this model more advanced approaches are required. The extended Fröhlich Hamiltonian has also been tackled in mean field studies [59, 102] that show how the energy gets shifted by many-polaron interactions. The mean field approaches show good agreement with the experiment which at first glance could be interpreted as an acceptable model. Unfortunately, this does not form a satisfying final theoretical explanation and a number of questions remain. More advanced beyond mean field theories such as RG or the path integral treatment in Chapter 3, tackling exactly the same models, show a significant shift further away from the experiment when compared to mean field approaches, as can for example be seen in Figures 3.4 and 3.5 of the previous chapter. The corrections obtained in mean field theories for the repulsive branch at very strong coupling, due to either many polaron effects or finite temperatures appear to be roughly of the same order as corrections from beyond mean field effects for a single polaron. In addition, it is reasonable to expect that higher-order phonon-phonon interactions could be of importance even in the regime where finite temperature mean field theory appears to work. This motivates the investigation of these phenomena in a beyond mean field theory for a complete picture. Some work in this direction can already be found. For example, the bound state between two polarons, the *bipolaron*, has been studied on the attractive branch [103] with effective Schrödinger equations and QMC methods. To the best of our knowledge no semi-analytical beyond mean field studies have been yet applied to study the many polaron properties beyond the Fröhlich model on the repulsive branch, which are of interest for future experiments.¹

For this reason, we are interested in generalizing the methods presented in Chapter 2 to describe the many polaron ground state using the general memory kernel method to also capture the interactions between the polarons. In the past, only limited interest existed for such general memory approaches because simple harmonic variational models, such as Feynman's original model action, were deemed already sufficient. Consequently, very few path integral techniques can be found in the literature that can be applied to many particle systems with general memory kernels.

In Chapter 2 we have presented a way to compute path integrals with general memory kernels for a single particle. A first possible step to generalize the approach is to consider a direct many particle extension of this method, which still forms a non-trivial task that we will return to. However, when dealing with multiple particles an additional question of accounting for particle statistics of identical particles arises. The impurities in the experiment of Aarhus [23] are bosons and it could be important to account for their statistics to describe the many polaron state. Although it is not implausible to assume that at low impurity densities at zero temperature the impurities could be approximated as distinguishable, it remains to be a question of interest to be able to confirm this in a more general approach. For this purpose, in the following two chapters we will develop a way to

¹Very recently, around the time this thesis was finalized, mean field and QMC results for many impurities in the full Bose polaron Hamiltonian have been obtained [104] which will form an important benchmark for future studies.

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perform path integrals for many particles in the presence of memory, and to be as general as possible also account for their identical nature. Although we will mainly focus on bosons, the extensions to fermions could be considered within the same framework. If it turns out that for bosons identical particle statistics play a small role in the ground state energy, we can always simply reduce the approach to the distinguishable particle case which still forms an interesting application that has not yet been studied in the literature. We start by providing some context for the techniques and methods used in this chapter.

4.1 Introduction

Since the initial proposal by Feynman [8], the variational path integral approach has known various extensions towards improving the model action or improvements towards other directions such as applications to multiple particles or entirely different physical systems than polarons [105, 106]. The former case has already been extensively discussed in Chapter 2, where we have shown that for more difficult impurity systems than the Fröhlich model it can be interesting to be able to extend the model action to a more general form than the commonly used coupled oscillator system as has been first proposed in [76, 77].

On the other hand extensions towards small numbers of multiple particles [97, 99] or even towards an arbitrary number of identical particles [98], have so far relied on using the types of restricted model actions that are constructed by integrating out harmonically coupled fictitious particles. Even in the absence of a fictitious system, the canonical ensemble treatment of identical particles in the path integral formalism significantly complicates the expressions for the partition and correlation functions [107, 108]. This naturally raises the question as to how these approaches could be extended to many identical particles using action functionals with general memory kernels, yielding an all encompassing treatment. In this chapter we answer the first part of this question by presenting a derivation of the partition function for such a general action functional. When necessary to emphasize that the memory kernels arise from the influence of an external system we will also refer to this quantity as the reduced partition function.

It is important to emphasize that in the context of variational models, the environment often plays merely the role of an intermediary used to obtain a variationally suitable expression for the retarded interactions. However, the thermodynamics that follows from the reduced partition function, interpreted as a

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toy model for an open quantum system, has been shown to display particularly interesting behavior in itself [109, 110]. As an example of an application we will show how our expression for the partition function with memory could provide a new angle towards the study of the specific heat for identical particles in this direction as well. Therefore, although the main motivation is to develop techniques that can be used for polaron physics, it will be worthwhile to pause and consider the thermodynamics following from these models as a standalone.

In this chapter we consider the following action functional (we will work in units of $\hbar = 1$) which forms a natural extension of the general model action in Chapter 2 (2.8):

$$S^{(N)}[\mathbf{\bar{r}}, x, y, \mathbf{\bar{\kappa}}] = \frac{m}{2} \sum_{i}^{N} \int_{0}^{\beta} \dot{\mathbf{r}}_{i}(\tau)^{2} d\tau + \frac{m}{2} \sum_{i}^{N} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\sigma x(\tau - \sigma) \mathbf{r}_{i}(\tau) \cdot \mathbf{r}_{i}(\sigma) + \frac{m}{2N} \sum_{i,j}^{N} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\sigma \left[y(\tau - \sigma) - x(\tau - \sigma) \right] \mathbf{r}_{i}(\tau) \cdot \mathbf{r}_{j}(\sigma) - m \sum_{i}^{N} \int_{0}^{\beta} d\tau \mathbf{r}_{i}(\tau) \cdot \mathbf{\kappa}_{i}(\tau).$$

$$(4.1)$$

For the functional arguments the notations $\bar{\mathbf{r}} = \mathbf{r}_1, ..., \mathbf{r}_N$ and $\bar{\mathbf{\kappa}} = \mathbf{\kappa}_1, ..., \mathbf{\kappa}_N$ are used. This (Euclidean) action functional describes N particles with mass m at temperature $(k_B\beta)^{-1}$, that interact through memory kernels $x(\tau - \sigma)$ and $y(\tau - \sigma)$. The memory kernels generally represent the effect of some external system or medium that induces retarded interactions, and would arise after integrating out the external system coupled to the particles. However, here they are taken to be completely general and can also be defined to include harmonic trapping potentials. One small difference with the definition in Chapter 2 is that here the memory kernels are defined with an additional factor β to present the same convention here as in the published version of this chapter [111]. To switch to the convention of Chapter 2 we merely would have to redefine the Fourier components $x_n \to \beta x_n$ at any point in the derivation later on.

In addition we introduce a set of completely general vector source functions $\kappa_i(\tau)$, which may represent time-dependent external forces on the particles, but will mainly prove to be useful for calculating expectation values. Expression (4.1) can be rewritten to note that each particle interacts with itself through the memory kernel $\frac{1}{N}((N-1)x(\tau-\sigma)+y(\tau-\sigma))$ and with any other particle through the memory kernel $\frac{1}{N}(y(\tau-\sigma)-x(\tau-\sigma))$, and hence the two can be tuned independently.

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We also restrict the memory kernels to be symmetric $(x(\tau), y(\tau)) = (x(-\tau), y(-\tau))$ and β -periodic $(x(\beta - \tau), y(\beta - \tau)) = (x(\tau), y(\tau))$. These are general properties of bosonic Green's functions [112] which are also assumed in the treatment for the single-polaron in [77], and naturally arise in systems with a harmonic coupling to an external system [48, 62, 81, 91, 97–99]. In addition we will assume that $\int_0^\beta x(\tau)d\tau \neq 0$ and $\int_0^\beta y(\tau)d\tau \neq 0$, so that we do not need to introduce a finite volume in our treatment - a technical step that occurs when taking the free particle limit as the harmonic oscillator frequency tends to zero. We specifically consider three dimensional systems and in further notation d = 3, unless specified otherwise.

The goal of this chapter is to obtain a recurrence relation for the partition function of bosons described by the general action functional (4.1). To provide an example of how our result can be applied to a specific choice of x and y, we also consider an application using the type of memory kernels occurring in harmonic systems [109]. Our approach generalizes the previously known calculations for a system of harmonically coupled identical oscillators in [107, 108], which correspond to a specific choice of memory kernels in (4.1). First, in Section 4.2 we will extend the calculation performed in [113] to a many-particle system to obtain the distinguishable particle propagator corresponding to Eq. (4.1). Next, in Section 4.3 we will discuss which steps of [107, 108] need to be generalized to take memory effects for identical particles into account. Therefore, in a way the results of this chapter can be seen as an application of the methods in [113] to generalize the approach in [107]. Finally, in Section 4.4 we will apply the results to consider the specific heat of an open quantum system of bosons, where the effects of the environment are represented by the memory kernels arising from a harmonic coupling to fictitious masses.

4.2 Propagator

Before taking the permutation symmetries of identical particles into account, first the many particle propagator for N distinguishable particles has to be calculated:

$$K_N[x, y, \overline{\kappa}](\overline{\mathbf{r}}_T, \beta | \overline{\mathbf{r}}_0, 0) = \int_{\overline{\mathbf{r}}_0, 0}^{\overline{\mathbf{r}}_T, \beta} \mathcal{D}\overline{\mathbf{r}} \ e^{-S^{(N)}[\overline{\mathbf{r}}, x, y, \overline{\kappa}]}.$$
(4.2)

The boundary points are indicated by $\overline{\mathbf{r}}_T = \overline{\mathbf{r}}(\beta)$ and $\overline{\mathbf{r}}_0 = \overline{\mathbf{r}}(0)$. To emphasize that the expression for the propagator is still a functional of the memory kernels and source functions, this dependence on x, y, and $\overline{\mathbf{\kappa}}$ is indicated in the square

brackets. The calculation of the propagator for N = 1 has been performed in [113], and we largely base our derivation for the many-particle case in the rest of this section on the methods presented in [113] and [107].

For a quadratic action functional given by expression (4.1), the path integral can be expanded around the classical paths that minimize the action functional to write:

$$K_N[x, y, \overline{\kappa}](\overline{\mathbf{r}}_T, \beta | \overline{\mathbf{r}}_0, 0) = K_N[x, y, \mathbf{0}](0, \beta | 0, 0) e^{-S_{\rm cl}[x, y, \overline{\kappa}](\overline{\mathbf{r}}_T, \overline{\mathbf{r}}_0)}.$$
(4.3)

Here, $S_{cl}[x, y, \overline{\kappa}](\overline{\mathbf{r}}_T, \overline{\mathbf{r}}_0)$ is the action functional (4.1) evaluated along the classical paths that are found as solutions to the following set of integro-differential equations:

$$\ddot{\mathbf{R}}(\tau) - \int_{0}^{\beta} y(\tau - \sigma) \mathbf{R}(\sigma) d\sigma + \mathbf{K}(\tau) = 0, \qquad (4.4)$$
$$\ddot{\mathbf{r}}_{i}(\tau) - \int_{0}^{\beta} x(t - \sigma) \mathbf{r}_{i}(\sigma) d\sigma - \int_{0}^{\beta} \left[y(\tau - \sigma) - x(\tau - \sigma) \right] \mathbf{R}(\sigma) d\sigma + \boldsymbol{\kappa}_{i}(\tau) = 0. \qquad (4.5)$$

The center of mass coordinate $\mathbf{R} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{r}_i$ decouples together with the center of mass source term $\mathbf{K} = \frac{1}{N} \sum_{i=1}^{N} \boldsymbol{\kappa}_i$ yielding an equation that has already been solved in [113]. Having obtained a solution to Eq. (4.4), the last two terms in Eq. (4.5) can be seen as an effective source term, which allows to solve Eq. (4.5) using the same approach. Substitution of the solutions into the action functional yields $S_{\rm cl}(\bar{\mathbf{r}}_T, \bar{\mathbf{r}}_0)$, which can then be used to derive the fluctuation factor $K_N[x, y, \mathbf{0}] (0, \beta | 0, 0)$ in the same way as in [113]. This lengthy calculation can be somewhat shortened by writing the paths in terms of fluctuations around the center of mass, for which the derivation is presented in Appendix D.

As shown in Appendix D, the many-body propagator (4.2) factorizes in terms of single-particle propagators just as in the case of a harmonically coupled system [107]:

$$K_{N}[x, y, \overline{\kappa}] (\overline{\mathbf{r}}_{T}, \beta | \overline{\mathbf{r}}_{0}, 0) = \frac{K[y, \sqrt{N}\mathbf{K}](\sqrt{N}\mathbf{R}_{T}, \beta | \sqrt{N}\mathbf{R}_{0}, 0)}{K[x, \sqrt{N}\mathbf{K}](\sqrt{N}\mathbf{R}_{T}, \beta | \sqrt{N}\mathbf{R}_{0}, 0)} \prod_{j=1}^{N} K[x, \kappa_{j}](\mathbf{r}_{j,T}, \beta | \mathbf{r}_{j,0}, 0).$$
(4.6)

The propagators on the right-hand side of Eq. (4.6) are the single particle propagators for which the action functional (4.1) depends on a single memory kernel, CHAPTER 4 - PATH INTEGRAL TECHNIQUES FOR MANY PARTICLES WITH GENERAL MEMORY

making the notation of Eq. (4.2) somewhat redundant. Hence, let us separately define the single particle propagator as a functional of only the memory kernel $x(\tau - \sigma)$:

$$K[x,\boldsymbol{\kappa}](\mathbf{r}_T,\beta|\mathbf{r}_0,0) = \int_{\mathbf{r}_0,0}^{\mathbf{r}_T,\beta} \mathcal{D}\mathbf{r} e^{-S^{(1)}[\mathbf{r},x,\boldsymbol{\kappa}]},$$
(4.7)

where:

$$S^{(1)}[\mathbf{r}, x, \boldsymbol{\kappa}] = \int_0^\beta \frac{m\dot{\mathbf{r}}^2}{2} dt + \frac{m}{2} \int_0^\beta d\tau \int_0^\beta d\sigma x(\tau - \sigma) \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma) - m \int_0^\beta d\tau \mathbf{r}(\tau) \cdot \boldsymbol{\kappa}(\tau).$$
(4.8)

In what follows, we will decompose the memory kernels and the source terms in their Fourier components x_n , y_n and κ_n , respectively, using the convention $f(\tau) = \sum_{n=-\infty}^{\infty} f_n e^{i\nu_n \tau}$, with $\nu_n = 2\pi n/\beta$ the bosonic Matsubara frequencies. Following the method of [113] and assuming the same stability conditions, we derive the following expression for the single-particle propagator with memory:

$$K[x, \boldsymbol{\kappa}](\mathbf{r}_{T}, \beta | \mathbf{r}_{0}, 0) = \left(\frac{m}{2\pi\beta}\right)^{d/2} \left(\frac{4}{\beta^{3}x_{0}\Delta_{x}}\right)^{d/2} \frac{1}{\prod_{k=1} \left(1 + \frac{\beta x_{k}}{\nu_{k}^{2}}\right)^{d}} \\ \times \exp\left[-\frac{m}{2\beta}A_{x}(\mathbf{r}_{T} - \mathbf{r}_{0})^{2} - \frac{m}{2\beta}\frac{1}{\Delta_{x}}(\mathbf{r}_{T} + \mathbf{r}_{0})^{2} \\ + \frac{2m}{\beta}\frac{1}{\Delta_{x}}\sum_{n}\frac{\boldsymbol{\kappa}_{n}}{\nu_{n}^{2} + \beta x_{n}} \cdot (\mathbf{r}_{T} + \mathbf{r}_{0}) \\ - \frac{2m}{\beta}\left(\frac{\beta}{2}\sum_{n\neq0}\frac{i\nu_{n}}{\nu_{n}^{2} + \beta x_{n}}\boldsymbol{\kappa}_{n}\right) \cdot (\mathbf{r}_{T} - \mathbf{r}_{0}) \\ - \frac{2m}{\beta}\frac{1}{\Delta_{x}}\left(\sum_{n}\frac{\boldsymbol{\kappa}_{n}}{\nu_{n}^{2} + \beta x_{n}}\right)^{2} + \frac{2m}{\beta}\left(\frac{\beta^{2}}{4}\sum_{n}\frac{\boldsymbol{\kappa}_{n} \cdot \boldsymbol{\kappa}_{-n}}{\nu_{n}^{2} + \beta x_{n}}\right)\right].$$

$$(4.9)$$

In Eq. (4.9) we have chosen a slightly different notation from [113] to define the following dimensionless functionals of the memory kernel x:

$$A_x = \sum_{n=-\infty}^{\infty} \frac{\beta x_n}{\nu_n^2 + \beta x_n},\tag{4.10}$$

$$\Delta_x = \frac{4}{\beta^2} \sum_{n=-\infty}^{\infty} \frac{1}{\nu_n^2 + \beta x_n}.$$
(4.11)

In what follows we will generally assume $A_x > 0$ and $\Delta_x > 0$ to restrict ourselves to
propagators (4.9) that are convergent for any combination of the boundary points. Note that due to the previous assumption of $x_0 \neq 0$ and $y_0 \neq 0$ the functionals are well-defined when written in this form. Nevertheless taking the limit $x_0, y_0 \rightarrow 0$ in the propagators still yields the appropriate expression, and this distinction will only become of importance in the partition function further on.

4.3 Partition function for identical particles with memory

The path-integral approach is naturally extended to the treatment of identical particles by taking all possible permutations of the end-points into account [62]. In this way, the canonical partition function for bosons is written as:

$$\mathcal{Z}(N) = \frac{1}{N!} \sum_{P} \int d\bar{\mathbf{r}} \int_{\bar{\mathbf{r}},0}^{P[\bar{\mathbf{r}}],\beta} \mathcal{D}\bar{\mathbf{r}}' \ e^{-S^{(N)}[\bar{\mathbf{r}}',x,y,\bar{\boldsymbol{\kappa}}]}.$$
(4.12)

The path integral counts all possible paths from an ordered set of initial points $\overline{\mathbf{r}} = {\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N}$ to a final set of points $P[\overline{\mathbf{r}}] = {P\mathbf{r}_1, P\mathbf{r}_2, ..., P\mathbf{r}_N}$ where the coordinates are reordered by a permutation P on a set of N, using the commonly used notation $P\mathbf{r}_1 = \mathbf{r}_{P(1)}$. All possible values of the set $\overline{\mathbf{r}}$ are then integrated out, and the sum over all possible permutations P is finally taken. The treatment can be straightforwardly extended to fermions by adding a factor $(-1)^P$ that provides a minus sign to all odd permutations.

The propagator (4.6) exhibits the same factorization pattern as a harmonically coupled system of oscillators, and hence initially the approach of [107] can be followed. The integration over all possible boundary points $\bar{\mathbf{r}}$ can be extended to include the center of mass variable through the introduction of a delta function,

$$\int d\mathbf{\bar{r}} \to \int d\mathbf{R} \int d\mathbf{\bar{r}} \,\,\delta\left(\mathbf{R} - \frac{1}{N}\sum_{i}\mathbf{r}_{i}\right),\tag{4.13}$$

which is then written in its Fourier representation [107]. This allows to separate the contribution of the center of mass propagators in Eq. (4.6) as follows:

$$\mathcal{Z}(N) = \frac{1}{(2\pi)^3} \int d\mathbf{k} \ \mathcal{Z}_R(N, \mathbf{k}) \mathcal{Z}_r(N, \mathbf{k}), \qquad (4.14)$$

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where:

$$\mathcal{Z}_R(N, \mathbf{k}) = \int d\mathbf{R} \ e^{i\mathbf{k}\cdot\mathbf{R}} \frac{K[y, \mathbf{0}](\sqrt{N}\mathbf{R}, \beta|\sqrt{N}\mathbf{R}, 0)}{K[x, \mathbf{0}](\sqrt{N}\mathbf{R}, \beta|\sqrt{N}\mathbf{R}, 0)},$$
(4.15)

and

$$\mathcal{Z}_{r}(N,\mathbf{k}) = \frac{1}{N!} \sum_{P} \int d\overline{\mathbf{r}} \prod_{j=1}^{N} K[x,\mathbf{0}](P\mathbf{r}_{j},\beta|\mathbf{r}_{j},0)e^{-i\mathbf{k}\cdot\mathbf{r}_{j}/N}.$$
 (4.16)

Note that we set the source functions $\kappa_i = 0$, as their main purpose was in deriving the fluctuation factor, and from now on we consider the action functional (4.1) without source terms. Following the standard approaches [62, 107], any permutation P can be partitioned into M_{ℓ} disjoint permutation cycles of length ℓ , which allows to write:

$$\mathcal{Z}_{r}(N,\mathbf{k}) = \sum_{M_{1},M_{2},\dots,M_{N}}^{*} \prod_{\ell=1}^{N} \frac{1}{\ell^{M_{\ell}}(M_{\ell})!} h_{\ell}(\mathbf{k})^{M_{\ell}}, \qquad (4.17)$$

where the * symbol above the summation symbol indicates a constrained summation that has to obey $\sum_{\ell=1}^{N} \ell M_{\ell} = N$. In this representation the nested *N*-dimensional integral in expression (4.16) factorizes as a product of ℓ -fold integrals that correspond to each permutation cycle:

$$h_{\ell}(\mathbf{k}) = \int d\mathbf{r}_{1} \dots \int d\mathbf{r}_{\ell} \ K[x, \mathbf{0}](\mathbf{r}_{1}, \beta | \mathbf{r}_{\ell}, 0) \dots K[x, \mathbf{0}](\mathbf{r}_{3}, \beta | \mathbf{r}_{2}, 0)$$
$$\times K[x, \mathbf{0}](\mathbf{r}_{2}, \beta | \mathbf{r}_{1} 0) e^{-i\frac{1}{N}\mathbf{k} \cdot \sum_{j=1}^{\ell} \mathbf{r}_{j}}.$$
(4.18)

The next step is to obtain an expression for $h_{\ell}(\mathbf{k})$, which requires the computation of a q-dimensional integral in expression (4.18). While high dimensional Gaussian integrals can always in principle be calculated by converting them into a linear algebra problem of finding a determinant of a ℓ -dimensional matrix, finding an explicit expression for the latter is not always equally straightforward. In the approach of [107] which we have thus far followed very closely, the integral (4.18) is calculated by relying on the composition property of the propagators. If the composition property holds, then $h_{\ell}(\mathbf{k})$ becomes the single-particle partition function of exactly the same system as described by the single-particle propagator, but at an inverse temperature $\ell\beta$ and with additional delta-kicks to account for the **k**-exponent. This partition function can then be readily computed with standard path integration methods. This trick is not applicable here, as the propagator with memory (4.9), does not obey the composition property. This can be easily seen by noting that the action functional (4.1) can not just be split into a sum of two parts on respective time intervals. In Appendix E we show how integral (4.18)can be directly computed and obtain the following result in d dimensions:

$$h_{\ell}(\mathbf{k}) = Q_x^{\ell d} \frac{1}{\left|2\sinh\left(\frac{\ell}{2}\operatorname{arccosh}\left[\frac{A_x\Delta_x+1}{A_x\Delta_x-1}\right]\right)\right|^d} \exp\left(-\frac{\ell k^2\beta}{8N^2m}\Delta_x\right),\tag{4.19}$$

where:

$$Q_x = \frac{1}{\prod_{k=1} \left(1 + \frac{\beta x_k}{\nu_k^2} \right)} \left(\frac{1}{\beta^3 x_0} \frac{4}{|A_x \Delta_x - 1|} \right)^{1/2}.$$
 (4.20)

The functional form of $h_{\ell}(\mathbf{k})$ is very similar to that found in [107]. The main differences are that the oscillator-frequency dependent parts are now replaced by expressions containing Δ_x and A_x , functionals of the memory kernel, appearing in the argument of the hyperbolic sine and the exponential. An additional factor Q_x appears, which equals 1 when the memory kernel x corresponds to a harmonic oscillator without memory.

The choice of writing expression (4.19) in terms of the hyperbolic sine has the advantage of being maximally illustrative in regards to how changes due to memory arise on top of previously known expressions in [107]. However, due to this choice some particular care should be taken when $\Delta_x A_x < 1$. In this case each of the two factors in the determinant (E.14) in Appendix E can become negative, and the complex modulus should be added after taking the square root if the factors are to be separated as in (4.19) and (4.20). For simple harmonic oscillator systems, and the model system considered in Section 4.4, $\Delta_x A_x > 1$ and this subtlety can be safely ignored.

The expression for the partition function (4.14) can now be computed. The center of mass $\mathcal{Z}_R(N, \mathbf{k})$ can be calculated from the propagators, and now that the **k**-dependence of $h_\ell(\mathbf{k})$ is known, the **k**-integral in (4.14) can be performed. After a some algebraic work one obtains:

$$\mathcal{Z}(N) = \mathbb{Z}(N)Q_x^{Nd} \left(\frac{\beta x_0}{\beta y_0}\right)^{d/2} \prod_{k=1}^{\infty} \left(\frac{1 + \frac{\beta x_k}{\nu_k^2}}{1 + \frac{\beta y_k}{\nu_k^2}}\right)^d .$$
(4.21)

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with \mathbb{Z} given by:

$$\mathbb{Z}(N) = \sum_{M_1, M_2, \dots, M_N}^* \prod_{\ell=1}^N \frac{1}{\ell^{M_\ell}(M_\ell)!} \frac{1}{\left|2\sinh\left(\frac{\ell}{2}\operatorname{arccosh}\left[\frac{A_x\Delta_x+1}{A_x\Delta_x-1}\right]\right)\right|^{M_\ell d}}.$$
 (4.22)

Note that due to the presence of the additional factor in expression (4.21) it is now the product $Q_x^{Nd}\mathbb{Z}(N)$ that represents the partition function in the absence of two-body interactions, extending the result of [107]. Following the approach in [107], the constrained summation (4.22) can be transformed into a recurrence relation as shown in Appendix F:

$$\mathbb{Z}(N) = \frac{1}{N} \sum_{k=0}^{N-1} \mathbb{Z}(k) \left| 2 \sinh\left[\frac{(N-k)}{2} \operatorname{arccosh}\left(\frac{A_x \Delta_x + 1}{A_x \Delta_x - 1}\right)\right] \right|^{-d}.$$
 (4.23)

The recurrence relation requires an initial value, and it can be seen that $\mathbb{Z}(0) = 1$ yields the correct $\mathcal{Z}(1)$ result according to expression (4.21). Alternatively, the factor Q_x could be absorbed in the definition of $\mathbb{Z}(N)$, but then the recurrence would have to start from $\mathbb{Z}(0) = Q_x^{Nd}$.

As a consistency check, consider the specific choice $x(\tau - \sigma) = w^2 \delta(\tau - \sigma)$ and $y(\tau - \sigma) = \Omega^2 \delta(\tau - \sigma)$ for which the action functional (4.1) exactly corresponds with the system of coupled oscillators in [107]. The different Matsubara sums and products in Eq. (4.21) can now be readily computed to find:

$$\left(\frac{\beta x_0}{\beta y_0}\right)^{d/2} \prod_{k=1}^{\infty} \left(\frac{1 + \frac{\beta x_k}{\nu_k^2}}{1 + \frac{\beta y_k}{\nu_k^2}}\right)^d = \frac{\sinh\left(\frac{\beta w}{2}\right)^d}{\sinh\left(\frac{\beta \Omega}{2}\right)^d},\tag{4.24}$$

and $Q_x = 1$. In particular, the resulting hyperbolic cosine from

$$\frac{A_x \Delta_x + 1}{A_x \Delta_x - 1} = \cosh(\beta w) \tag{4.25}$$

allows to cancel the inverse hyperbolic cosine in the weight factor of the recurrence relation (4.23). Substituting these results, the expression for the partition function in [107] is exactly retrieved in this limit.



4.4 - Example application: open quantum system of identical oscillators

FIGURE 4.1: A one dimensional depiction of the system described by (4.26).

4.4 Example application: open quantum system of identical oscillators

In this chapter we present a brief example application of the derived expressions to a stylized model of an open quantum system of identical particles. We consider a system of N of non-interacting bosonic oscillators in a harmonic trap with frequency Ω . As depicted in Figure 4.1, the effect of some environment is then represented as the presence of memory kernels that arise from integrating out fictitious harmonically coupled particles with mass M and frequency W. The thermodynamics of systems in such an environment have been studied for distinguishable particles in [114, 115]. Note that because of the Bose statistics that have to be imposed, this model is more than simply N unrelated copies of a single oscillator with memory.

To obtain an expression for the memory kernels, the fictitious particles are taken to be uncoupled and distinguishable, which could represent an environment with a far slower relaxation than the bosonic system. Consider the (Euclidean) Lagrangian of the full system corresponding to the partition function Z_{tot} of the system depicted in Figure 4.1:

$$L_{\text{tot}} = \sum_{i=1}^{N} \left(\frac{m}{2} \dot{\mathbf{r}}_{i}^{2} + \frac{m\Omega^{2}}{2} \mathbf{r}_{i}^{2} + \frac{M}{2} \dot{\mathbf{Q}}_{i}^{2} + \frac{MW^{2}}{2} (\mathbf{r}_{i} - \mathbf{Q}_{i})^{2} \right),$$
(4.26)

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and the Lagrangian of the external system is defined as:

$$L_{\rm f} = \sum_{i=1}^{N} \left(\frac{M}{2} \dot{\mathbf{Q}}_i^2 + \frac{MW^2}{2} \mathbf{Q}_i^2 \right).$$
(4.27)

It is important to note that through (4.27) we adopt the view of the external system as defined in [109]. The external system is considered to be the whole of the fictitious particles and springs with constant MW^2 that are attached to the degrees of freedom of interest. The fictitious particles can be integrated out as in [48] to obtain the reduced partition function:

$$\mathcal{Z}(N) = \frac{\mathcal{Z}_{\text{tot}}(N)}{\mathcal{Z}_f(N)},\tag{4.28}$$

where Z_f is the partition function of the external system corresponding to (4.27). Expression (4.28) appears to be exactly the identical particle extension of one of the stylized models of an open quantum system considered in [109]. The resulting Z(N) can now be cast in the form of (4.12), where the memory kernels in the action functional (4.1) are given by:

$$x(\tau-\sigma) = y(\tau-\sigma) = \frac{MW^2}{m} \left[\frac{W^2 + \frac{m}{M}\Omega^2}{W^2} \delta(\tau-\sigma) - \frac{W\cosh(W\left[|\tau-\sigma|-\beta/2\right])}{2\sinh(W\beta/2)} \right].$$
(4.29)

This is the simplest translationally non-invariant model that provides a memory kernel $x(\tau - \sigma)$ with non-trivial memory effects for the recurrence relation (4.23). Having obtained an explicit expression for the memory kernels of interest, we proceed to illustrate how our formalism can be applied.

The functionals A_x and Δ_x are obtained after computing the Matsubara summations in expressions (4.10) and (4.11):

$$A_x = \frac{\beta\omega_+}{2} \coth\left(\frac{\beta\omega_+}{2}\right)\gamma_+ + \frac{\beta\omega_-}{2} \coth\left(\frac{\beta\omega_-}{2}\right)\gamma_-, \qquad (4.30)$$

$$\Delta_x = \frac{2}{\beta\omega_+} \coth\left(\frac{\beta\omega_+}{2}\right) \gamma_+ + \frac{2}{\beta\omega_-} \coth\left(\frac{\beta\omega_-}{2}\right) \gamma_-, \qquad (4.31)$$

where:

$$\omega_{\pm}^{2} = \frac{\frac{m+M}{m}W^{2} + \Omega^{2} \pm \sqrt{\left(\frac{m+M}{m}W^{2} + \Omega^{2}\right)^{2} - 4W^{2}\Omega^{2}}}{2}, \qquad (4.32)$$

4.4 - Example application: open quantum system of identical oscillators

$$\gamma_{\pm} = \frac{1}{2} \left[1 \pm \frac{\Omega^2 + \left(\frac{M}{m} - 1\right) W^2}{\omega_+^2 - \omega_-^2} \right].$$
(4.33)

The frequencies ω_{\pm} that diagonalize the full system [109] therefore naturally appear in the calculation.

Since for this system $y_n = x_n$, the interaction factor in front of (4.21) cancels out and the partition function $\mathcal{Z}(N)$ is written as a product of only two factors, Q_x^{Nd} and the recurrence part $\mathbb{Z}(N)$. The Matsubara product in (4.20) can be computed for the specific memory kernel (4.29), which allows to write:

$$Q_x = \frac{2\sinh\left(\frac{\beta W}{2}\right)}{\beta W} \frac{\beta \omega_+}{2\sinh\left(\frac{\beta \omega_+}{2}\right)} \frac{\beta \omega_-}{2\sinh\left(\frac{\beta \omega_-}{2}\right)} \left(\frac{1}{\beta^3 x_0} \frac{4}{\Delta_x A_x - 1}\right)^{1/2}, \quad (4.34)$$

with Δ_x and A_x known from (4.31) and (4.30). In three dimensions the recurrence relation (4.23) for $\mathbb{Z}(N)$ has no known solution, and has to be computed numerically. As shown in the approach of [107] a numerically stable implementation is obtained by defining:

$$b = e^{-q}, \qquad q = \operatorname{arccosh}\left[\frac{\Delta_x A_x + 1}{\Delta_x A_x - 1}\right],$$
(4.35)

and without loss of generality proposing the following way of writing the recurrence factor:

$$\mathbb{Z}(N) = \prod_{j=1}^{N} \rho_j \frac{b^{\frac{3}{2}}}{(1-b^j)^3}.$$
(4.36)

This fixes the first coefficient $\rho_1 = 1$, and after substitution of (4.36) into (4.23) a recurrence relation for ρ_N is found:

$$\rho_N = \frac{1}{N} \frac{\left(1 - b^N\right)^3}{\left(1 - b\right)^3} \left[1 + \sum_{k=0}^{N-2} \frac{(1 - b)^3}{\left(1 - b^{(N-k)}\right)^3} \prod_{j=k+1}^{N-1} \frac{(1 - b^j)^3}{\rho_j} \right].$$
(4.37)

Due to the additional factor in the expression for the partition function $\mathcal{Z}(N) = Q_x^{Nd}\mathbb{Z}(N)$, the internal energy and specific heat of the system are written as a sum of two terms:

$$U(N) = U_Q(N) + \mathbb{U}(N) = -3N\partial_\beta \log(Q_x) - \partial_\beta \log(\mathbb{Z}), \qquad (4.38)$$

$$C(N) = C_Q(N) + \mathbb{C}(N) = 3Nk_B\beta^2\partial_\beta^2\log(Q_x) + k_B\beta^2\partial_\beta^2\log(\mathbb{Z}).$$
(4.39)

Analytical expressions for U_Q and \mathcal{C}_Q can straightforwardly be calculated from

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the factor Q_x in (4.34). The recurrence relations for $\mathbb{U}(N)$ and $\mathbb{C}(N)$ are obtained after computing the partial derivatives of $\log(\mathbb{Z})$ by combining (4.36) with (4.37):

$$\frac{\mathbb{U}(N)}{\partial_{\beta}q} = \frac{1}{N} \frac{1}{\rho_N} \frac{(1-b^N)^3}{(1-b)^3} \left(\frac{\mathbb{U}(N-1)}{\partial_{\beta}q} + \frac{3}{2} \frac{1+b}{1-b} + \sum_{k=0}^{N-2} \frac{(1-b)^3}{(1-b^{(N-k)})^3} \left[\frac{\mathbb{U}(k)}{\partial_{\beta}q} + \frac{3(N-k)}{2} \frac{1+b^{(N-k)}}{1-b^{(N-k)}} \right] \prod_{j=k+1}^{N-1} \frac{(1-b^j)^3}{\rho_j} ,$$
(4.40)

and

$$\mathbb{C}(N)k_B^{-1} = \frac{1}{N}\sum_{k=0}^{N-1} \frac{1}{(1-b^{(N-k)})^3} \prod_{j=k+1}^N \frac{(1-b^j)^3}{\rho_j} \left(k_B^{-1}\mathbb{C}(k) + \beta^2 \left[\frac{3(N-k)}{2}\frac{1+b^{(N-k)}}{1-b^{(N-k)}}\partial_\beta q + \mathbb{U}(k) - \mathbb{U}(N)\right] \left[\frac{3(N-k)}{2}\frac{1+b^{(N-k)}}{1-b^{(N-k)}}\partial_\beta q + \mathbb{U}(k)\right] + \beta^2 3(N-k)^2 \frac{b^{(N-k)}}{(1-b^{(N-k)})^2} (\partial_\beta q)^2 - \beta^2 \frac{3(N-k)}{2}\frac{1+b^{(N-k)}}{1-b^{(N-k)}}\partial_\beta^2 q\right).$$
(4.41)

Here, the recurrence formulas are initiated from $\mathbb{U}(0) = 0$ and $\mathbb{C}(0) = 0$, and the partial derivatives $\partial_{\beta}q$ and ∂_{β}^2q can be analytically computed from (4.35) since Δ and A are known.

The specific heat (4.39) is shown in Figure 4.2 as a function of the temperature, measured with respect to the critical temperature in the absence of the external system $k_B T_c = \hbar \Omega \left(N/\zeta(3) \right)^{1/3}$, with $\zeta(x)$ the Riemann zeta function. We can clearly observe the main bosonic condensation peak slightly below the critical temperature, which at weak coupling to the environment corresponds exactly to the result in [107]. The sharpness of the peak fades towards stronger coupling with the external system but nevertheless remains visibly present. In addition to the main condensation peak, at an intermediate coupling strength an anomalous dip and peak are observed at low temperatures. These anomalous features in the specific heat of open quantum systems have been studied for a distinguishable particles in [109, 115, 116], where it is shown that the specific heat can even become negative for certain systems. It is explained in [109, 115] by the fact that the specific heat (4.39) is the difference of the specific heats of the system and the trapped fictitious particles as defined in the partition function (4.28), and a more extensive interpretation can be found in [116].

We can also note that the high and low temperature limits of the specific



FIGURE 4.2: Specific heat per particle as a function of the temperature of N = 100 non-interacting bosons in a harmonic potential coupled to an environment of harmonically coupled fictitious particles with M = m. The results are shown for three coupling strengths $W = [0.01\Omega, 4\Omega, 10\Omega]$ plotted by respectively the dashed, filled and dotted lines.

heat are in agreement with [115]. From expression (4.34) we can see that at high temperatures for $\beta \to 0$, Q_x approaches a finite value and hence the first part of the specific heat $C_Q(N)$ in (4.39) goes to zero. In the same limit the recurrence part of the partition function can be shown to diverge as $\mathbb{Z} \sim \beta^{-dN}$, from which follows $C(N) = 3Nk_B$. In the low-temperature limit $\beta \to \infty$ one can show that in the presence of the environment \mathbb{Z} remains finite, and Q_x becomes an exponential function of β , from which follows C(N) = 0.

An overview of the structure of the main condensation peak and the anomalous dip is presented in Figure 4.3. For both a light and heavy mass M of the fictitious particles, remnants of the bosonic condensation peak remain visible up to strong coupling with the external system. At low temperatures and weaker coupling the anomalous dip can be seen as region of lighter shading. Contrary to the single particle case for this system [109], we find that the anomalous dip can drop below zero for bosons in Figure 4.3 where the dashed loop indicates a region of negative specific heat.

As can also be seen from Figure 4.3, coupling with the external system significantly lowers the effective critical temperature of the bosons. This can be understood by noting that the generalized bosonic recurrence relation (4.23) is CHAPTER 4 - PATH INTEGRAL TECHNIQUES FOR MANY PARTICLES WITH GENERAL MEMORY

nothing else than the recurrence relation for harmonically trapped bosons where the trap frequency is replaced by a temperature-dependent quantity:

$$\tilde{\Omega}(T) = \frac{1}{\beta} \operatorname{arccosh} \left[\frac{\Delta_x A_x + 1}{\Delta_x A_x - 1} \right], \qquad (4.42)$$

which allows to define an effective critical temperature as the solution of:

$$\frac{\tilde{T}_c}{T_c} = \frac{\tilde{\Omega}(\tilde{T}_c)}{\Omega}.$$
(4.43)

The results are plotted as the dotted lines on Figure 4.3 and agree well with the behavior of the condensation peak. It is important to note that only the recurrence part is correctly reproduced by substituting $\Omega \to \tilde{\Omega}(T)$ in the harmonic oscillator result. The factor Q_x in front of the partition function (4.21) is not retrieved this way because it is entirely absent in the harmonic case. As the latter however can be taken out of the recurrence relation it is no surprise that it should play no significant role in the inherently bosonic features of the system, and the behavior of the condensation peak is accurately reproduced by (4.43). The constant difference between (4.43) and the condensation peak in Figure 4.3 is readily explained by the fact that finite-particle effects have not been accounted for in the definition of T_c .

4.5 Conclusion

In this chapter we presented an approach that extends previous methods of computing path integrals for identical particles to action functionals with general memory kernels. First, the many-body propagator for distinguishable particles was derived and shown to exhibit the same factorization pattern in terms of singleparticle propagators as seen in harmonically coupled systems without retardation [107]. However, the main difference is that the single-particle propagators no longer obey the composition property when the system has memory. This complicates the computation of a class of integrals appearing in the derivation of the partition function, for which we obtain explicit expressions by utilizing the properties of circulant matrices. The resulting expression for the partition function is a functional applicable to a general class of memory kernels, and is shown to reduce to the known result for harmonically coupled systems without memory in the appropriate limit.

As an illustration of the method to a specific choice of memory kernels, the



FIGURE 4.3: The color map of the specific heat per particle $C/(k_BN)$ for N = 500 bosons, for (a) M = m and (b) M = 10m. The dashed loop in the bottom left corner indicates the region where the specific heat becomes negative. The dotted line indicates the effective temperature obtained from (4.43).

results were then applied to study the specific heat of non-interacting bosons in a harmonic trap in the presence of memory kernels that arise from harmonic couplings to fictitious particles. This provides the simplest model system that yields non-trivial memory effects in the condensation recurrence relation. We show that the presence of the environment shifts the bosonic condensation to lower temperatures and significantly smooths out the Bose condensation peak in the specific heat, which nevertheless remains visible even at strong coupling. To better understand these types of open systems, and in particular to calculate the density and the pair correlation functions, expressions for the identical particle one-and two point generating functionals are required, which will be the focus of the next chapter.

CHAPTER 5

Path integral techniques for many particles with general memory: Correlation functions

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In the previous chapter, the results of which can also be found in [111], the partition sum and some derived thermodynamic quantities such as the internal energy and the specific heat were calculated. However, for a more complete picture and variational applications it is necessary to also know the one-and two-point correlation functions. These quantities give access to expectation values of single-particle operators (such as the density) and of two-body operators (such as the pair correlation function). The goal of the current chapter is to derive the one-particle reduced density matrix and the two-point correlation function. As an example, we then apply these results to the same open quantum system of bosons coupled to a model environment of distinguishable masses as discussed in Chapter 4.

In Sec. 5.1, a short review of previously obtained results is presented, and the path-integral definitions of the one-particle reduced density matrix and the two-point correlation function are given. We calculate expressions for the former in Sec. 5.2, and for the latter in Sec. 5.3. The obtained result for the two-point

correlation function provides a generalization of expressions found in [108] to systems with memory. Our result for the one-particle reduced density matrix allows for the computation of the effective states and occupation numbers of the bosons. In Sec. 5.4 we apply these results to further explore the simplified model of bosons in an environment introduced in Chapter 4 and in particular focus on the behavior of density and condensate fraction. Conclusions are drawn in Sec. 5.5.

5.1 Quadratic many-body systems with memory

In Chapter 4 the distinguishable particle propagator corresponding to the general memory action functional (4.1) was computed in (4.6). In this chapter we will be relying on these results and using the same notation with minor additions. It will further on be useful to separately define the fluctuation factor in front of the single-particle propagator (4.9) as:

$$\mathcal{A} = \left(\frac{m}{2\pi\beta}\right)^{1/2} \left(\frac{4}{\beta^3 x_0 \Delta_x(0)}\right)^{1/2} \prod_{k=1} \left(1 + \frac{\beta x_k}{\nu_k^2}\right)^{-1}.$$
 (5.1)

Note that we will also be using the shorthand notation for the single particle propagator $K[x] = K[x, \mathbf{0}]$ further on, corresponding to setting all κ_n to zero in expression (4.9), which leaves just the first two terms in the exponent. In contrast to expression (4.11) of the previous chapter we will now require a time-dependent $\Delta(\tau)$ and hence the dimensionless functionals A_x and $\Delta_x(\tau)$ appearing in the propagator are defined as:

$$A_x = \sum_{n=-\infty}^{\infty} \frac{\beta x_n}{\nu_n^2 + \beta x_n},\tag{5.2}$$

$$\Delta_x(\tau) = \frac{4}{\beta^2} \sum_{n=-\infty}^{\infty} \frac{e^{i\nu_n \tau}}{\nu_n^2 + \beta x_n}.$$
(5.3)

We will use the shorthand notation $\Delta_x = \Delta_x(0)$ and in general we will assume $A_x > 0$ and $\Delta_x > 0$ in this chapter to restrict the memory kernels to produce bounded propagators as a function of the end-points (4.9).

Let us write the partition function of a system of bosons described by (4.1) as $\mathcal{Z}[\overline{\kappa}](N)$, where the dependence on the source functions is explicitly highlighted in the functional. In Chapter 4 the partition function $\mathcal{Z}(N) = \mathcal{Z}[\mathbf{0}](N)$ for this system without source terms, $\overline{\kappa} = \mathbf{0}$, was calculated in (4.21) and applied to study the specific heat of a model of an open quantum system. The goal of this chapter is to expand upon this calculation and derive expressions for the one-particle reduced density matrix (from which the one-point correlation function readily follows) and the two-point correlation function. The one-particle reduced density matrix is computed in a similar way as the partition function in Chapter 4, but now the integration variable \mathbf{r}_1 is removed from the integral resulting in an N-1dimensional integral over $\tilde{\mathbf{r}} = {\mathbf{r}_2, ..., \mathbf{r}_N}$, and in the boundary points of the path integral \mathbf{r}_1 is replaced by respectively \mathbf{r} and $\mathbf{r'}$:

$$\rho_1(\mathbf{r}'|\mathbf{r}) = \frac{1}{\mathcal{Z}(N)} \frac{1}{N!} \sum_P \int d\mathbf{\tilde{r}} \int_{\{\mathbf{r},\mathbf{r}_2,\dots,\mathbf{r}_N\},0}^{P[\{\mathbf{r}',\mathbf{r}_2,\dots,\mathbf{r}_N\}],\beta} \mathcal{D}\mathbf{\bar{r}}'' e^{-S^{(N)}[\mathbf{\bar{r}}'',x,y,\mathbf{0}]}.$$
 (5.4)

For the computation of the two-point correlation function, the structure of the path-integral is somewhat simpler as all variables $\bar{\mathbf{r}} = {\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N}$ are treated on the same footing, but an additional weighing factor containing two different variables \mathbf{r}_1 and \mathbf{r}_2 (identical for any $i \neq j$) appears:

$$\left\langle e^{i\mathbf{q}\cdot(\mathbf{r}_{1}(\tau)-\mathbf{r}_{2}(\sigma))}\right\rangle_{I} = \frac{1}{\mathcal{Z}(N)} \frac{1}{N!} \sum_{P} \int d\mathbf{\bar{r}} \int_{\mathbf{\bar{r}},0}^{P[\mathbf{\bar{r}}],\beta} \mathcal{D}\mathbf{\bar{r}}' \ e^{i\mathbf{q}\cdot(\mathbf{r}_{i}(\tau)-\mathbf{r}_{j}(\sigma))} e^{-S^{(N)}[\mathbf{\bar{r}}',x,y,\mathbf{0}]}.$$
(5.5)

In the next two sections, we perform the many-body path integrations in expressions (5.4) and (5.5).

5.2 One-particle reduced density matrix

The derivation of the one-particle reduced density matrix can be summarized as a modification of the derivation of the partition function in Chapter 4, now to account for the unequal treatment of the variables \mathbf{r} and $\mathbf{r'}$ in comparison to the other variables $\tilde{\mathbf{r}} = {\mathbf{r}_2, ..., \mathbf{r}_N}$. The first step is to note that for any fixed permutation, the path integral in (5.4) is given by the propagator (4.6), where the center of mass part is unaffected by the permutations while the rest of the end points have to be permuted accordingly. The center of mass can now be isolated in the same spirit as in [107, 111] using a modified variable $\tilde{\mathbf{R}} = \frac{1}{N} \sum_{j=2}^{N} \mathbf{r}_j$ that only contains integration variables. This allows us to write:

$$\rho_1(\mathbf{r}'|\mathbf{r}) = \frac{1}{(2\pi)^d} \frac{1}{\mathcal{Z}(N)} \int d\mathbf{k} \ \mathcal{P}_{\tilde{R}}(N, \mathbf{k}) \mathcal{P}_r(N, \mathbf{k}), \tag{5.6}$$

where the center of mass contribution is the Gaussian integral:

$$\mathcal{P}_{\tilde{R}}(N,\mathbf{k}) = \int d\mathbf{\tilde{R}} \ e^{i\mathbf{k}\cdot\mathbf{\tilde{R}}} \frac{K[y]\left(\sqrt{N}\mathbf{\tilde{R}} + \frac{1}{\sqrt{N}}\mathbf{r},\beta|\sqrt{N}\mathbf{\tilde{R}} + \frac{1}{\sqrt{N}}\mathbf{r}',0\right)}{K[x]\left(\sqrt{N}\mathbf{\tilde{R}} + \frac{1}{\sqrt{N}}\mathbf{r},\beta|\sqrt{N}\mathbf{\tilde{R}} + \frac{1}{\sqrt{N}}\mathbf{r}',0\right)},\tag{5.7}$$

which is readily computed if we assume that $\Delta_x > \Delta_y$. The remaining factor contains the permutations:

$$\mathcal{P}_{r}(N,\mathbf{k}) = \frac{1}{N!} \sum_{P} \int d\mathbf{\tilde{r}} K[x] \left(\mathbf{r}_{P(N)}, \beta | \mathbf{r}_{N}, 0 \right) \dots K[x] \left(\mathbf{r}', \beta | \mathbf{r}_{j}, 0 \right)$$
$$\times \dots K[x] \left(\mathbf{r}_{P(1)}, \beta | \mathbf{r}, 0 \right) e^{-i\mathbf{k} \cdot \sum_{j=2}^{N} \mathbf{r}_{j}/N}, \qquad (5.8)$$

where P(n) represents the element that ends up at the position of n after the permutation on the ordered set $\{1, 2, ..., N\}$. Expression (5.8) illustrates how the end-point \mathbf{r}' of the one-particle reduced density matrix is permuted to some position j, while the initial point \mathbf{r} remains in place and gets coupled with element P(1).



FIGURE 5.1: Example of a cyclic decomposition for N = 5 where the arrows represent the single-particle propagators (4.9). The cyclic decomposition of the partition function in the absence of source terms, as performed in the previous chapter, is illustrated in (a) where the closed cycles contribute a factor $h_{\ell}(\mathbf{k})$ given by (5.10). The modified decomposition of the one body reduced density matrix $\rho_1(\mathbf{r}'|\mathbf{r})$ is shown in (b), where one cycle is now opened up contributing a factor $O_{\ell}(\mathbf{k})$ in (5.9) while the remaining points are still partitioned in terms of closed cycles.

We now follow the standard approach [62, 107, 111] to decompose the summation of permutations in (5.8) in terms of its cyclic decomposition, an argument which will require some modification for the calculation of ρ_1 . It is easy to see that most cycles will be completely unaffected by the presence of **r** and **r'** and will yield exactly the same contribution $h_{\ell}(\mathbf{k})$ as computed for the partition function in expression (4.19) of Chapter 4. In fact, there will be only one modified permutation chain starting at $\mathbf{r} \to \mathbf{r}_{P(1)} \to \dots$ that has to end at \mathbf{r}' . As illustrated in Figure 5.1, this chain can be thought of as an open cycle with length ℓ the contribution of which we will call $O_{\ell}(\mathbf{k})$. The summation in (5.8) can therefore be written as the summation over all the possible open cycles $O_{\ell}(\mathbf{k})$ multiplied with the cyclic decomposition on the remaining $N - \ell$ points (and taking the combinatorics into account):

$$\mathcal{P}_{r}(N,\mathbf{k}) = \frac{1}{N} \sum_{\ell=1}^{N} O_{\ell}(\mathbf{k}) \sum_{M_{1},\dots,M_{N-\ell}}^{*} \prod_{n=1}^{N-\ell} \frac{h_{n}(\mathbf{k})^{M_{n}}}{n^{M_{n}}M_{n}!}.$$
(5.9)

Here, M_n is the number of cycles of length n in the decomposition and \sum^* represents the constraint $\sum_n M_n = N - \ell$. The ordinary closed cycles $h_n(\mathbf{k})$ were computed in expression (4.19) of Chapter 4:

$$h_{\ell}(\mathbf{k}) = Q_x^{\ell d} \frac{1}{\left[2\left|\sinh\left(\frac{\ell}{2}\operatorname{arccosh}\left[\frac{A_x\Delta_x+1}{A_x\Delta_x-1}\right]\right)\right|\right]^d} \exp\left(-\frac{\ell k^2\beta}{8N^2m}\Delta_x\right), \qquad (5.10)$$

with:

$$Q_x = \frac{1}{\prod_{k=1} \left(1 + \frac{\beta x_k}{\nu_k^2} \right)} \left(\frac{1}{\beta^3 x_0} \frac{4}{|A_x \Delta_x - 1|} \right)^{1/2},$$
(5.11)

and the open cycles are given by:

$$O_{\ell}(\mathbf{k}) = \int d\mathbf{r}_{2} \dots \int d\mathbf{r}_{\ell} \ K[x](\mathbf{r}',\beta|\mathbf{r}_{\ell},0) \dots K[x](\mathbf{r}_{3},\beta|\mathbf{r}_{2},0)$$
$$\times K[x](\mathbf{r}_{2},\beta|\mathbf{r},0)e^{-\frac{i\mathbf{k}}{N}\cdot\sum_{j=2}^{\ell}\mathbf{r}_{j}}.$$
(5.12)

This integral is computed in Appendix G and is shown to be equal to:

$$O_{\ell}(\mathbf{k}) = \mathcal{A}^{\ell d} \left(\frac{\pi^{\ell-1}}{\left[\frac{m}{2\beta} \left(A_x - \frac{1}{\Delta_x}\right)\right]^{\ell-1} U_{\ell-1}(\zeta)} \right)^{d/2} \\ \times \exp\left(-\frac{\beta k^2}{8N^2 m} \Delta_x \left[\ell - \sqrt{A_x \Delta_x} \tanh\left(\frac{\ell}{2} \operatorname{arccosh}(\zeta)\right)\right] \\ - \frac{i\mathbf{k}}{2N} \cdot (\mathbf{r} + \mathbf{r}') \left[\sqrt{A_x \Delta_x} \tanh\left(\frac{\ell}{2} \operatorname{arccosh}(\zeta)\right) - 1\right]$$

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$$-\frac{m}{\beta}\sqrt{\frac{A_x}{\Delta_x}}\tanh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)(\mathbf{r}^2+\mathbf{r}'^2)-\frac{m}{\beta}\sqrt{\frac{A_x}{\Delta_x}}\frac{1}{\sinh(\ell\operatorname{arccosh}(\zeta))}(\mathbf{r}-\mathbf{r}')^2\right),\tag{5.13}$$

where

$$\zeta = \frac{A_x \Delta_x + 1}{A_x \Delta_x - 1},\tag{5.14}$$

and $U_{\ell-1}$ is a Chebyshev polynomial of the second kind defined in expression (G.6) of Appendix G for $|\zeta| > 1$.

The closed cycles $h_n(\mathbf{k})$ (5.10) can be now substituted in (5.9) after which the Fourier integral in (5.6) can be readily performed. The final expression for the one particle reduced density matrix is found as:

$$\rho_{1}(\mathbf{r}'|\mathbf{r}) = \left(\frac{2m}{\pi\beta}\right)^{d/2} \frac{1}{N} \sum_{\ell=1}^{N} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} \left(\frac{1}{\left[\sqrt{\frac{\Delta_{x}}{A_{x}}} \coth\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right) - \frac{1}{N}(\Delta_{x} - \Delta_{y})\right]}\right)^{d/2} \frac{1}{\left|2\sinh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)\right|^{d}} \exp\left(-\frac{m}{\beta}\sqrt{\frac{A_{x}}{\Delta_{x}}} \tanh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)(\mathbf{r}^{2} + \mathbf{r}'^{2})\right)\right) \exp\left(-\frac{m}{2\beta}\frac{\frac{1}{N}(\Delta_{x} - \Delta_{y})\sqrt{\frac{A_{x}}{\Delta_{x}}}}{\sqrt{\frac{\Delta_{x}}{\Delta_{x}}}} \tanh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)}(\mathbf{r} + \mathbf{r}')^{2}\right)\right) \exp\left(-\frac{m}{2\beta}\left[\frac{1}{N}(A_{y} - A_{x}) + \sqrt{\frac{A_{x}}{\Delta_{x}}}\frac{2}{\sinh(\ell\operatorname{arccosh}(\zeta))}\right](\mathbf{r} - \mathbf{r}')^{2}\right).$$
(5.15)

Here, $\mathbb{Z}(N)$ can be found as the solution to the recurrence relation (with $\mathbb{Z}(0) = 1$) studied in the previous chapter:

$$\mathbb{Z}(N) = \frac{1}{N} \sum_{k=0}^{N-1} \mathbb{Z}(k) \frac{1}{\left|2\sinh\left(\frac{(N-k)}{2}\operatorname{arccosh}(\zeta)\right)\right|^d}.$$
(5.16)

Note that by relabeling $k = N - \ell$ it follows from (5.16) that for any N:

$$\frac{1}{N} \sum_{\ell=1}^{N} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} \frac{1}{\left|2\sinh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)\right|^d} = 1,$$
(5.17)

which guarantees that the one-particle reduced density matrix (5.15) is always

5.3 - Two-point correlation function

normalized.

The diagonal of ρ_1 in position space can be readily taken and yields the average boson density $n(\mathbf{r}) = \rho_1(\mathbf{r}|\mathbf{r})$. Note that here and in the rest of this chapter the density will be normalized to 1 rather than to N:

$$n(\mathbf{r}) = \left(\frac{2m}{\pi\beta}\right)^{d/2} \frac{1}{N} \sum_{\ell=1}^{N} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} \left(\frac{1}{\left[\sqrt{\frac{\Delta_x}{A_x}} \coth\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right) - \frac{1}{N}(\Delta_x - \Delta_y)\right]}\right)^{d/2} \times \frac{1}{\left|2\sinh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)\right|^d} \exp\left(-\frac{2m}{\beta} \frac{1}{\sqrt{\frac{\Delta_x}{A_x}} \coth\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right) - \frac{1}{N}(\Delta_x - \Delta_y)} \mathbf{r}^2\right).$$
(5.18)

We can now consider a specific choice of memory kernels $x(\tau - \sigma) = \omega^2 \delta(\tau - \sigma)$ and $y(\tau - \sigma) = \Omega^2 \delta(\tau - \sigma)$ in which case the action functional (4.1) reduces to that of a system of harmonically trapped bosons all coupled by springs, as studied in [108]. In this case the Matsubara summations (5.2) and (5.3) can be computed to find $\Delta_x = \frac{2}{\beta\omega} \coth\left(\frac{\beta\omega}{2}\right)$, $\Delta_y = \frac{2}{\beta\Omega} \coth\left(\frac{\beta\Omega}{2}\right)$ and $A_x = \frac{\beta\omega}{2} \coth\left(\frac{\beta\omega}{2}\right)$. In addition $\zeta = \cosh\left(\frac{\beta\omega}{2}\right)$ which nicely cancels with the arccosh function in the argument of the hyperbolic sine. After substitution in (5.18), the expression for the density in [108] is retrieved exactly.

5.3 Two-point correlation function

Let us now introduce the notation $\overline{\kappa}_2 = (\kappa_1, \kappa_2, 0, ...)$, where the overline in $\overline{\kappa}_2$ indicates it being a vector of vectors, whereas κ_2 is merely one of its components. The goal of this section is to find an expression for the partition function with two general non-zero source terms

$$\mathcal{Z}[\overline{\kappa}_2](N) = \frac{1}{N!} \sum_P \int d\overline{\mathbf{r}} \int_{\overline{\mathbf{r}},0}^{P[\overline{\mathbf{r}}],\beta} \mathcal{D}\overline{\mathbf{r}}' \ e^{-S^{(N)}[\overline{\mathbf{r}}',x,y,\overline{\kappa}_2]},\tag{5.19}$$

which after division by $\mathcal{Z}(N)$ and setting $\kappa_1(\tau') = \frac{i\mathbf{q}}{m}\delta(\tau - \tau')$ and $\kappa_2(\sigma') = -\frac{i\mathbf{q}}{m}\delta(\sigma - \sigma')$ yields exactly the two point correlation function (5.5). First, the propagator (4.6) is substituted in (5.19) where two source terms are set non-zero. Contrary to the approach in Section 5.2, all of the variables $\mathbf{\bar{r}}$ are integrated out in (5.19). The center of mass can therefore be separated using the complete CM

variables $\mathbf{R} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{r}_i$ and $\mathbf{K}_2 = \frac{1}{N} (\boldsymbol{\kappa}_1 + \boldsymbol{\kappa}_2)$ which allows to write:

$$\mathcal{Z}[\overline{\kappa}_2](N) = \frac{1}{(2\pi)^d} \int d\mathbf{k} \ \mathcal{Z}_R[\overline{\kappa}_2](N, \mathbf{k}) \mathcal{Z}_r[\overline{\kappa}_2](N, \mathbf{k}), \tag{5.20}$$

where:

$$\mathcal{Z}_{R}[\overline{\kappa}_{2}](N,\mathbf{k}) = \int d\mathbf{R} \, \frac{K[y,\sqrt{N}\mathbf{K}_{2}](\sqrt{N}\mathbf{R},\beta|\sqrt{N}\mathbf{R},0)}{K[x,\sqrt{N}\mathbf{K}_{2}](\sqrt{N}\mathbf{R},\beta|\sqrt{N}\mathbf{R},0)},\tag{5.21}$$

and:

$$\mathcal{Z}_{r}[\overline{\boldsymbol{\kappa}}_{2}](N,\mathbf{k}) = \frac{1}{N!} \sum_{P} \int d\overline{\mathbf{r}} \ e^{-\frac{i\mathbf{k}}{N} \cdot \sum_{j=1}^{N} \mathbf{r}_{j}} \prod_{j=3}^{N} K[x](P\mathbf{r}_{j},\beta|\mathbf{r}_{j},0) \\ \times K[x,\boldsymbol{\kappa}_{2}](P\mathbf{r}_{2},\beta|\mathbf{r}_{2},0)K[x,\boldsymbol{\kappa}_{1}](P\mathbf{r}_{1},\beta|\mathbf{r}_{1},0).$$
(5.22)

In expression (5.22) all source functions are set to zero except for the two sources κ_1 and κ_2 corresponding to the propagators starting in initial points \mathbf{r}_1 and \mathbf{r}_2 . Making use of expression (4.9) for the propagator, (5.22) can also be written as:

$$\mathcal{Z}_{T}[\overline{\boldsymbol{\kappa}}_{2}](N,\mathbf{k}) = \frac{1}{N!} e^{-S_{c1}^{(1)}[x,\boldsymbol{\kappa}_{1}](0,0) - S_{c1}^{(1)}[x,\boldsymbol{\kappa}_{2}](0,0)} \sum_{P} \int d\overline{\mathbf{r}} \ e^{-\frac{i\mathbf{k}}{N} \cdot \sum_{j=1}^{N} \mathbf{r}_{j}} \\ \times e^{\tilde{\mathbf{a}}_{1}(P\mathbf{r}_{1}+\mathbf{r}_{1}) + \tilde{\mathbf{b}}_{1}(P\mathbf{r}_{1}-\mathbf{r}_{1})} e^{\tilde{\mathbf{a}}_{2}(P\mathbf{r}_{2}+\mathbf{r}_{2}) + \tilde{\mathbf{b}}_{2}(P\mathbf{r}_{2}-\mathbf{r}_{2})} \prod_{j=1}^{N} K[x](P\mathbf{r}_{j},\beta|\mathbf{r}_{j},0),$$

$$(5.23)$$

where the path-independent contribution of the propagators was taken out of the integral by using the notation:

$$S_{\rm cl}^{(1)}\left[x,\boldsymbol{\kappa}\right](0,0) = \frac{2m}{\beta} \frac{1}{\Delta_x(0)} \left(\sum_n \frac{\boldsymbol{\kappa}_n}{\nu_n^2 + \beta x_n}\right)^2 - \frac{2m}{\beta} \left(\frac{\beta^2}{4} \sum_n \frac{\boldsymbol{\kappa}_n \cdot \boldsymbol{\kappa}_{-n}}{\nu_n^2 + \beta x_n}\right).$$
(5.24)

In addition we define the short-hand notation for the linear terms in the exponent corresponding to the two source terms s = 1, 2:

$$\tilde{\mathbf{a}}_{\mathbf{s}} = \frac{2m}{\beta} \frac{1}{\Delta_x(0)} \sum_n \frac{\boldsymbol{\kappa}_{\mathbf{s},n}}{\nu_n^2 + \beta x_n}, \qquad \tilde{\mathbf{b}}_{\mathbf{s}} = -\frac{2m}{\beta} \left(\frac{\beta}{2} \sum_{n \neq 0} \frac{i\nu_n}{\nu_n^2 + \beta x_n} \boldsymbol{\kappa}_{\mathbf{s},n} \right).$$
(5.25)

The approach to compute (5.23) is once again to decompose the permutation in terms of cycles just as in [108, 111] or Section 5.2, with some modifications.

Consider any general permutation on N points out of the summation in (5.23).

For $2 \leq \ell \leq N$ there will be $N - \ell$ points that form cycles that do not pass through either \mathbf{r}_1 or \mathbf{r}_2 and yield the ordinary closed cycle contributions $h_n(\mathbf{k})$ as given in (5.10). To account for the cycle(s) on the remaining ℓ points, the set of all permutations has to be partitioned into two classes. In one class of permutations, the points \mathbf{r}_1 or \mathbf{r}_2 will lie in two disjoint cycles of respectively length ℓ and $\ell - j$ with $1 \leq j \leq \ell - 1$. We will call the contributions of each of those cycles $H_{\ell}^{(1)}(\mathbf{k})$ and $H_{\ell-j}^{(2)}(\mathbf{k})$ which are structurally similar to the ordinary closed cycle $h_n(\mathbf{k})$, but now contain the special points \mathbf{r}_1 or \mathbf{r}_2 due to the non-zero source term $\overline{\kappa}_2$. In this first class of permutations the contribution of the two cycles can therefore be written as a product $H_j^{(1)}(\mathbf{k})H_{\ell-j}^{(2)}(\mathbf{k})$. In the second class of permutations, those points will be in the same cycle of length ℓ and yield a single contribution $\chi_\ell(\mathbf{k}, j')$ which also depends on the distance between the two points j' within this cycle, with $1 \leq j' \leq \ell - 1$. After taking the combinatorics into account, this result is written down as:

$$\mathcal{Z}_{r}[\overline{\kappa}_{2}](N,\mathbf{k}) = \frac{e^{-S_{cl}^{(1)}[x,\kappa_{1}](0,0) - S_{cl}^{(1)}[x,\kappa_{2}](0,0)}}{N(N-1)} \left[\sum_{\ell=2}^{N} \sum_{j=1}^{\ell-1} H_{j}^{(1)}(\mathbf{k}) H_{\ell-j}^{(2)}(\mathbf{k}) \right] \\ \times \sum_{M_{1},\dots,M_{N-\ell}}^{*} \prod_{n=1}^{N-\ell} \frac{h_{n}(\mathbf{k})^{M_{n}}}{n^{M_{n}}M_{n}!} + \sum_{\ell=2}^{N} \sum_{j'=1}^{\ell-1} \chi_{\ell}(\mathbf{k},j') \sum_{M_{1},\dots,M_{N-\ell}}^{*} \prod_{n=1}^{N-\ell} \frac{h_{n}(\mathbf{k})^{M_{n}}}{n^{M_{n}}M_{n}!} \right], \quad (5.26)$$

and after relabeling the integration variables we can write for n = 1, 2:

$$H_{\ell}^{(n)}(\mathbf{k}) = \int d\mathbf{r}_{1} \dots \int d\mathbf{r}_{\ell} \ e^{\mathbf{\tilde{a}_{n}}(\mathbf{r}_{2}+\mathbf{r}_{1})+\mathbf{\tilde{b}_{n}}(\mathbf{r}_{2}-\mathbf{r}_{1})} K[x](\mathbf{r}_{1},\beta|\mathbf{r}_{\ell},0) \dots$$

$$\times K[x](\mathbf{r}_{2},\beta|\mathbf{r}_{1}0)e^{-\frac{i\mathbf{k}}{N}\cdot\sum_{j=1}^{\ell}\mathbf{r}_{j}},$$
(5.27)

and:

$$\chi_{\ell}(\mathbf{k},j) = \int d\mathbf{r}_{1} \dots \int d\mathbf{r}_{\ell} \ e^{\tilde{\mathbf{a}}_{1}(\mathbf{r}_{2}+\mathbf{r}_{1})+\tilde{\mathbf{b}}_{1}(\mathbf{r}_{2}-\mathbf{r}_{1})} K[x](\mathbf{r}_{1},\beta|\mathbf{r}_{\ell},0) \dots K[x](\mathbf{r}_{2},\beta|\mathbf{r}_{1}0)$$
$$e^{-\frac{i\mathbf{k}}{N} \cdot \sum_{j=1}^{\ell} \mathbf{r}_{j}} e^{\tilde{\mathbf{a}}_{2}(\mathbf{r}_{j+2}+\mathbf{r}_{j+1})+\tilde{\mathbf{b}}_{2}(\mathbf{r}_{j+2}-\mathbf{r}_{j+1})}. \tag{5.28}$$

In Appendix H expressions for both types of cycles are derived. If the notation from Appendix H is used, $a = \frac{m}{2\beta}A_x$, $b = \frac{m}{2\beta}\frac{1}{\Delta x}$, to keep the expressions compact,

the cycles can be written as:

$$H_{\ell}^{(n)}(\mathbf{k}) = Q_{x}^{\ell d} \frac{1}{\left[2\left|\sinh\left(\frac{\ell}{2}\operatorname{arccosh}\left(\zeta\right)\right)\right|\right]^{d}} \exp\left(-\frac{\ell k^{2}}{16N^{2}b} - \frac{i\mathbf{k}\cdot\tilde{\mathbf{a}}_{\mathbf{n}}}{4Nb}\right) + \frac{\tilde{\mathbf{a}}_{\mathbf{n}}^{2}a - \tilde{\mathbf{b}}_{\mathbf{n}}^{2}b}{a - b} \frac{1}{4\sqrt{ab}} \coth\left(\frac{\ell}{2}\operatorname{arccosh}\left(\zeta\right)\right) - \frac{1}{4}\frac{\tilde{\mathbf{a}}_{\mathbf{n}}^{2} - \tilde{\mathbf{b}}_{\mathbf{n}}^{2}}{a - b}\right), \quad (5.29)$$

and:

$$\chi_{\ell}(\mathbf{k}, j) = Q_x^{\ell d} \frac{1}{\left[2 \left| \sinh\left(\frac{\ell}{2} \operatorname{arccosh}\left(\zeta\right)\right) \right| \right]^d} \\ \times \exp\left(\frac{-\ell k^2}{16N^2 b} - \frac{i\mathbf{k}}{4Nb} \cdot \left(\mathbf{\tilde{a}_1} + \mathbf{\tilde{a}_2}\right) + \frac{1}{4} \left(\mathbf{\tilde{a}_1}^2 + \mathbf{\tilde{b}_1}^2 + \mathbf{\tilde{a}_2}^2 + \mathbf{\tilde{b}_2}^2\right) D_0 \\ + \frac{1}{4} \left(\mathbf{\tilde{a}_1}^2 - \mathbf{\tilde{b}_1}^2 + \mathbf{\tilde{a}_2}^2 - \mathbf{\tilde{b}_2}^2\right) D_1 + \frac{1}{2} \left(\mathbf{\tilde{a}_1} \cdot \mathbf{\tilde{a}_2} + \mathbf{\tilde{b}_1} \cdot \mathbf{\tilde{b}_2}\right) D_j \\ + \frac{1}{4} (\mathbf{\tilde{a}_1} - \mathbf{\tilde{b}_1}) \cdot (\mathbf{\tilde{a}_2} + \mathbf{\tilde{b}_2}) D_{j+1} + \frac{1}{4} (\mathbf{\tilde{a}_1} + \mathbf{\tilde{b}_1}) \cdot (\mathbf{\tilde{a}_2} - \mathbf{\tilde{b}_2}) D_{j-1} \right), \qquad (5.30)$$

where:

$$D_{\ell}(n) = \frac{1}{2\sqrt{ab}} \frac{\cosh\left[\left(\frac{\ell}{2} - n\right)\operatorname{arccosh}\left(\zeta\right)\right]}{\sinh\left(\frac{\ell}{2}\operatorname{arccosh}\left(\zeta\right)\right)}.$$
(5.31)

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All that remains now is to compute the Gaussian integral in the center of mass part (5.21), and then combine the resulting expression with (5.26) to compute the Fourier integral in (5.20). Although a rather lengthy calculation, it is reliant only on basic Gaussian integrals and goniometric identities, and we proceed to the final result:

$$\frac{\mathcal{Z}[\overline{\kappa}_{2}](N)}{\mathcal{Z}(N)} = \frac{1}{N(N-1)} e^{-\tilde{S}[\overline{\kappa}_{2}]} \sum_{\ell=2}^{N} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} h_{\ell}(\mathbf{0}) Q_{x}^{-\ell d} \sum_{j=1}^{\ell-1} \left[\frac{h_{j}(\mathbf{0})h_{\ell-j}(\mathbf{0})}{h_{\ell}(\mathbf{0})} \times \exp\left(-\frac{2m}{\beta} \frac{1}{\sqrt{A_{x}\Delta_{x}}} \left[\mathcal{J}[\kappa_{1},\kappa_{1}] \coth\left(\frac{j}{2} \operatorname{arccosh}(\zeta)\right) \right] \right) + \mathcal{J}[\kappa_{2},\kappa_{2}] \coth\left(\frac{\ell-j}{2} \operatorname{arccosh}(\zeta)\right) \right] \right) + \exp\left(-\frac{2m}{\beta} \frac{1}{\sqrt{A_{x}\Delta_{x}}} \left[\mathcal{J}[\kappa_{1},\kappa_{1}] + \mathcal{J}[\kappa_{2},\kappa_{2}] \right] \coth\left(\frac{\ell}{2} \operatorname{arccosh}(\zeta)\right) - \frac{4m}{\beta} \frac{1}{\sqrt{A_{x}\Delta_{x}}} \right] \mathcal{J}[\kappa_{1},\kappa_{2}] \frac{\cosh\left(\left[\frac{\ell}{2}-j\right] \operatorname{arccosh}(\zeta)\right)}{\sinh\left(\frac{\ell}{2} \operatorname{arccosh}(\zeta)\right)} - \frac{4m}{\beta} \mathcal{X}[\kappa_{1},\kappa_{2}] \frac{\sinh\left(\left[\frac{\ell}{2}-j\right] \operatorname{arccosh}(\zeta)\right)}{\sinh\left(\frac{\ell}{2} \operatorname{arccosh}(\zeta)\right)} \right] \right) \tag{5.32}$$

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Here the functionals of the two source terms $(\alpha, \gamma = 1, 2)$ in the exponents of the cycle-dependent contributions are given by:

$$\mathcal{J}[\boldsymbol{\kappa}_{\alpha},\boldsymbol{\kappa}_{\gamma}] = -\frac{1}{A_{x}\Delta_{x}-1} \left[A_{x} \left(\sum_{n} \frac{\boldsymbol{\kappa}_{\alpha,n}}{\nu_{n}^{2}+\beta x_{n}} \right) \left(\sum_{n} \frac{\boldsymbol{\kappa}_{\gamma,n}}{\nu_{n}^{2}+\beta x_{n}} \right) -\Delta_{x} \left(\frac{\beta}{2} \sum_{n\neq 0} \frac{i\nu_{n}}{\nu_{n}^{2}+\beta x_{n}} \boldsymbol{\kappa}_{\alpha,n} \right) \cdot \left(\frac{\beta}{2} \sum_{n\neq 0} \frac{i\nu_{n}}{\nu_{n}^{2}+\beta x_{n}} \boldsymbol{\kappa}_{\gamma,n} \right) \right], \quad (5.33)$$

$$\mathcal{X}[\boldsymbol{\kappa}_{1},\boldsymbol{\kappa}_{2}] = -\frac{1}{A_{x}\Delta_{x}-1} \left[\sum_{n} \frac{\boldsymbol{\kappa}_{1,n}}{\nu_{n}^{2}+\beta x_{n}} \cdot \left(\frac{\beta}{2} \sum_{n \neq 0} \frac{i\nu_{n}}{\nu_{n}^{2}+\beta x_{n}} \boldsymbol{\kappa}_{2,n} \right) - \sum_{n} \frac{\boldsymbol{\kappa}_{2,n}}{\nu_{n}^{2}+\beta x_{n}} \cdot \left(\frac{\beta}{2} \sum_{n \neq 0} \frac{i\nu_{n}}{\nu_{n}^{2}+\beta x_{n}} \boldsymbol{\kappa}_{1,n} \right) \right], \quad (5.34)$$

and the argument of the cycle-independent exponent in front is given by:

$$\tilde{S}[\overline{\kappa}_{2}] = -\frac{(N-1)m\beta}{2N} \sum_{n} \frac{\kappa_{1,n} \cdot \kappa_{1,-n} + \kappa_{2,n} \cdot \kappa_{2,-n}}{\nu_{n}^{2} + \beta x_{n}}$$

$$- \frac{m\beta}{2N} \sum_{n} \frac{\kappa_{1,n} \cdot \kappa_{1,-n} + \kappa_{2,n} \cdot \kappa_{2,-n}}{\nu_{n}^{2} + \beta y_{n}}$$

$$+ \frac{m\beta}{2N} \sum_{n} \frac{2\kappa_{1,n} \cdot \kappa_{2,-n}}{\nu_{n}^{2} + \beta x_{n}} - \frac{m\beta}{2N} \sum_{n} \frac{2\kappa_{1,n} \cdot \kappa_{2,-n}}{\nu_{n}^{2} + \beta y_{n}} - \frac{2m}{\beta} \left[\mathcal{J}[\kappa_{1},\kappa_{1}] + \mathcal{J}[\kappa_{2},\kappa_{2}] \right].$$
(5.35)

Expression (5.32) is precisely $\left\langle \exp\left(m\int_{0}^{\beta}d\tau_{1}\left(\mathbf{r}_{1}(\tau_{1})\boldsymbol{\kappa}_{1}(\tau_{1})+\mathbf{r}_{2}(\tau_{1})\boldsymbol{\kappa}_{2}(\tau_{1})\right)\right)\right\rangle$ with the expectation value taken with respect to the unsourced system. To obtain the two-point correlation function (5.5) we set the two source functions equal to respectively $\mathbf{f}_{1}(\tau_{1}) = \frac{i\mathbf{q}}{m}\delta(\tau_{1}-\tau)$ and $\mathbf{f}_{2}(\tau_{2}) = -\frac{i\mathbf{q}}{m}\delta(\tau_{2}-\sigma)$, which leaves the general form of expression (5.32) unchanged except for simplifying the functionals \mathcal{J}, \mathcal{X} and \tilde{S} to:

$$\mathcal{J}[\mathbf{f}_1, \mathbf{f}_1] = \frac{q^2 \beta^2}{16m^2} \frac{1}{A_x \Delta_x - 1} \left[A_x \Delta_x(\tau)^2 - \Delta_x \left(\frac{\beta}{2} \partial_\tau \Delta_x(\tau)\right)^2 \right],\tag{5.36}$$

$$\mathcal{J}[\mathbf{f}_2, \mathbf{f}_2] = \frac{q^2 \beta^2}{16m^2} \frac{1}{A_x \Delta_x - 1} \left[A_x \Delta_x(\sigma)^2 - \Delta_x \left(\frac{\beta}{2} \partial_\sigma \Delta_x(\sigma)\right)^2 \right],\tag{5.37}$$

$$\mathcal{J}[\mathbf{f}_{1},\mathbf{f}_{2}] = -\frac{q^{2}\beta^{2}}{16m^{2}}\frac{1}{A_{x}\Delta_{x}-1}\left[A_{x}\Delta_{x}(\tau)\Delta_{x}(\sigma) - \Delta_{x}\left(\frac{\beta}{2}\partial_{\tau}\Delta_{x}(\tau)\right)\left(\frac{\beta}{2}\partial_{\sigma}\Delta_{x}(\sigma)\right)\right],$$

$$(5.38)$$

$$\mathcal{X}[\mathbf{f}_{1},\mathbf{f}_{2}] = \frac{q^{2}\beta^{2}}{16m^{2}}\frac{1}{A_{x}\Delta_{x}-1}\left[\Delta_{x}(\tau)\left(\frac{\beta}{2}\partial_{\sigma}\Delta_{x}(\sigma)\right) - \Delta_{x}(\sigma)\left(\frac{\beta}{2}\partial_{\tau}\Delta_{x}(\tau)\right)\right],$$

$$(5.39)$$

$$\tilde{S}[\overline{\kappa}_{2}] = \frac{q^{2}\beta}{4mN} \left[(N-1)\Delta_{x} + \Delta_{y} + \Delta_{x}(\tau-\sigma) - \Delta_{y}(\tau-\sigma) \right] - \frac{2m}{\beta} \left[\mathcal{J}[\mathbf{f}_{1}, \mathbf{f}_{1}] + \mathcal{J}[\mathbf{f}_{2}, \mathbf{f}_{2}] \right].$$
(5.40)

Note that in (5.36)-(5.40) the full time-dependence of $\Delta_x(\tau)$ as defined in (5.3) is invoked, but for the purpose of keeping the expressions shorter we will use $\Delta_x = \Delta_x(0)$ in the case of $\tau = 0$, as has also been done in the rest of this section. Although (5.32) has no closed form expression, the numerical solution mainly requires knowing the factor $\mathbb{Z}(N)$, which is obtained by solving (5.16) as shown in [111] or Chapter 4. Finally, just as considered in Section 5.2 for the density, the coupled harmonic oscillator limit of the two-point correlation function can be checked for $\tau = \sigma = 0$, and exactly agrees with the results in [108].

5.4 Example application: density and pair correlation functions in an open quantum system

In this section, as a further illustration of the method, the expressions derived in Sections 5.2 and 5.3 are applied to study the particle density, condensed fraction and two-point correlations of a system of bosons in a model environment proposed in Chapter 4. To recap, consider N non-interacting bosonic oscillators labeled by the coordinates $\overline{\mathbf{r}} = {\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N}$, coupled to a set of external distinguishable masses labeled by $\overline{\mathbf{Q}} = {\mathbf{Q}_1, \mathbf{Q}_2, ..., \mathbf{Q}_N}$, where the total system is described by the previously introduced Lagrangian in (4.26):

$$L_{\text{tot}} = \sum_{i=1}^{N} \left(\frac{m}{2} \dot{\mathbf{r}}_{i}^{2} + \frac{m\Omega^{2}}{2} \mathbf{r}_{i}^{2} + \frac{M}{2} \dot{\mathbf{Q}}_{i}^{2} + \frac{MW^{2}}{2} \left(\mathbf{r}_{i} - \mathbf{Q}_{i} \right)^{2} \right).$$
(5.41)

The bosons with mass m are trapped in a harmonic potential with frequency Ω . The environment is modeled by integrating out the fictitious masses to obtain the 5.4 - Example application: density and pair correlation functions in an open quantum system

memory kernels at the level of the action functional (4.1):

$$x(\tau-\sigma) = y(\tau-\sigma) = \frac{MW^2}{m} \left[\frac{W^2 + \frac{m}{M}\Omega^2}{W^2} \delta(\tau-\sigma) - \frac{W\cosh(W\left[|\tau-\sigma|-\beta/2\right])}{2\sinh(W\beta/2)} \right].$$
(5.42)

In the rest of this section only equal masses M = m will be considered, and W/Ω will be used as the coupling parameter to the environment.

Note that contrary to the treatment in the previous chapter, every expression studied in this section follows from expectation values, and there is no necessity to explicitly define the external system relative to which the energy would be measured. Having obtained the memory kernels (5.42) for this system, expressions for Δ_x , A_x , Q_x and $\mathbb{Z}(N)$ can be computed and were discussed in Chapter 4. Since for the two-point correlation functions we will restrict ourselves to equal times $\tau = \sigma = 0$, this is sufficient to compute any of the quantities from Section 5.2 and 5.3. Note that for this particular system we have numerically checked that $\Delta_x A_x > 1$ and hence $\zeta > 1$, which restricts the use of all inverse hyperbolic functions to their real domain and allows us to drop the absolute value signs.

Before proceeding to the presentation of the results let us consider the oneparticle reduced density matrix which simplifies quite a bit in the x = y case as per (5.42):

$$\rho_{1}(\mathbf{r}'|\mathbf{r}) = \left(\frac{2m}{\pi\beta}\right)^{d/2} \frac{1}{N} \sum_{\ell=1}^{N} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} \left(\sqrt{\frac{A_{x}}{\Delta_{x}}} \tanh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)\right)^{d/2}$$
$$\frac{1}{\left|2\sinh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)\right|^{d}} \exp\left(-\frac{m}{\beta}\sqrt{\frac{A_{x}}{\Delta_{x}}} \tanh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)(\mathbf{r}^{2} + \mathbf{r}'^{2})\right)$$
$$-\frac{m}{\beta}\sqrt{\frac{A_{x}}{\Delta_{x}}} \frac{1}{\sinh(\ell \operatorname{arccosh}(\zeta))}(\mathbf{r} - \mathbf{r}')^{2}\right).$$
(5.43)

In general, the one-particle reduced density matrix (5.43) describes a mixed state at the single particle level due to entanglement with the rest of the system and can be decomposed in terms of a classical ensemble with occupation numbers. In Appendix I we show how the spectral decomposition of (5.43) is obtained (in d = 3):

$$\rho_1(\mathbf{r}'|\mathbf{r}) = \sum_{n_x, n_y, n_z}^{\infty} \lambda_{\mathbf{n}} \psi_{\mathbf{n}}^*(\mathbf{r}) \psi_{\mathbf{n}}(\mathbf{r}'), \qquad (5.44)$$

with the effective eigenstates and occupancy numbers given by:

$$\psi_{\mathbf{n}}(\mathbf{r}) = \mathcal{N}_{\mathbf{n}} H_{n_x} \left(\sqrt{\alpha} x \right) H_{n_y} \left(\sqrt{\alpha} y \right) H_{n_z} \left(\sqrt{\alpha} z \right) \exp\left(-\alpha \mathbf{r}^2 \right), \tag{5.45}$$

$$\lambda_{\mathbf{n}} = \frac{1}{N} \sum_{\ell=1}^{N} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} e^{-\left(\frac{1}{2} + n_x + n_y + n_z\right)\ell} \operatorname{arccosh}(\zeta), \qquad (5.46)$$

where H_n is a Hermite polynomial, \mathcal{N}_n is the normalization factor of the eigenstate, and $\alpha = \frac{2m}{\beta} \sqrt{\frac{A_x}{\Delta_x}}$.



FIGURE 5.2: The occupation numbers at $T/T_c = 0.01$ (T_c defined as the condensation temperature for N = 100 at W = 0) of the ground state and the first excited state (counting degeneracy) for respectively N = 1 and N = 100, are shown as a function of W, the strength of the coupling to the bath of distinguishable particles.

In Figure 5.2 the occupation numbers of the effective ground state and first excited state are compared for respectively N = 100 bosons and for N = 1, of which the latter is equivalent to the distinguishable particle case of the system. The results are plotted as a function of the coupling W between the bosons and the bath. For numerical purposes the temperature is taken to be finite $T/T_c = 0.01$, where $k_B T_c = \hbar \Omega (N/\zeta(3))^{1/3}$ for N = 100. In practice this represents the T = 0 case as the results have already converged as a function of temperature. At W = 0 and T = 0 each particle can be described by the same pure $\lambda_0 = 1$ harmonic oscillator ground-state $\psi_0(\mathbf{r})$ regardless of the particles being distinguishable or not. This should not be surprising as in the $T \to 0$ limit the ground state of N distinguishable non-interacting particles also obeys the bosonic permutation

symmetry. However, as W is increased, the N = 1 case rapidly loses its purity as the excited states of the density matrix spike in their occupancy numbers. Bosons, on the other hand, retain a macroscopic occupation of the ground state up to far stronger coupling strengths, illustrating how condensation could protect the system from entanglement with the environment.



FIGURE 5.3: Panel (a) presents the central density of N = 100 bosons (normalized by its value in the absence of the environment) for a series of low temperatures as a function of W. In panel (b) the spatial profile of the ground state is shown at zero temperature (normalized by its maximum value in the absence of an environment) for a set of coupling strengths W. The height of the shaded region in the peak relative to the peak height represents the occupation number λ_0 . This also indicates the central density of the ground state fraction as this quantity is proportional to λ_0 .

The ground state $\psi_0(\mathbf{r})$ gets more sharply peaked when W is increased as can be seen from (5.45), which combined with the behavior of λ_0 leads to a peculiar behavior of the particle density (5.18). As can be seen in Figure 5.3a, the central density of the bosonic cloud obtains a non-monotonic behavior as a function of Wat low temperatures. The origin of this behavior is revealed in Figure 5.3b: the initial increase in central density as a function of W is due to the compression of the condensate wave function, whereas the subsequent decrease when W is further increased is due to the depletion of the condensate, as depletion overtakes the compression effect on the condensate wave function.

In the previous discussion we assume that the central density closely mirrors the condensate central density. This is a qualitative argument that neglects the

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FIGURE 5.4: The density radial profile (a) and the pair correlation function (b) of N = 100 bosons for a series of coupling strengths W at a temperature $T = 0.4T_c$. The square scatters indicate the asymptotic model results given by (5.48) and (5.49).

contribution from the excited states compared to the ground state. In contrast to the bosonic case, distinguishable particles do not retain a macroscopic occupation of the ground state and there the central density is determined by the excited states. In this case the above argument will no longer hold which makes the behavior in Figure 5.3 uniquely bosonic. We can also consider the radial profile of the density n(r) shown in Figure 5.4a where the non-monotonic behavior is clearly visible.

Having obtained an expression for the two-point correlation function (5.32), we can compute the radial pair correlation function representing the average density around each particle as [108]:

$$g(r) = \frac{N-1}{(2\pi)^d} \int \mathbf{dq} \left\langle e^{i\mathbf{q}\cdot(\mathbf{r}_1(0) - \mathbf{r}_2(0))} \right\rangle e^{-i\mathbf{q}\cdot\mathbf{r}}.$$
 (5.47)

The radial profile of this correlation function is shown in Figure 5.4b and qualitatively looks nearly identical to the average density profiles. This is to be expected since g(r) is still a measure for the particle density, only now conditional to a boson being present at $\mathbf{r} = 0$. The most noticeable difference is that at strong coupling W, the pair correlation exhibits a sharp spike at small distances.

To understand this, it is illustrative to discuss the strong coupling limit of this model. Since the external particles in (5.41) are distinguishable, taking $W \to \infty$

effectively glues them to the bosons giving them a distinguishable label as depicted in Figure 5.5. As a reminder, we are considering the equal masses case M = m, and hence in this limit we should be able to describe the total system as a gas of distinguishable non-interacting composite particles with mass $\tilde{m} = 2m$ that are harmonically trapped by a frequency $\tilde{\Omega} = \Omega/\sqrt{2}$. The density of such a system is readily written down as the diagonal of the normalized propagator of the harmonic oscillator with mass \tilde{m} and frequency $\tilde{\Omega}$:

$$\tilde{n}(\mathbf{r},T) = \left(\frac{\sqrt{2}m\Omega\tanh\left(\frac{\beta\Omega}{2\sqrt{2}}\right)}{\pi}\right)^{d/2} \exp\left(-\sqrt{2}m\Omega\tanh\left(\frac{\beta\Omega}{2\sqrt{2}}\right)\mathbf{r}^2\right).$$
(5.48)

If the particles are distinguishable and non-interacting the pair correlation function \tilde{g} of this asymptotic model can be computed as:

$$\tilde{g}(\mathbf{r},T) = (N-1) \int \mathbf{dr}' \tilde{n}(\mathbf{r}',T) \tilde{n}(\mathbf{r}'+\mathbf{r},T)$$

$$= (N-1) \left(\frac{m\Omega \tanh\left(\frac{\beta\Omega}{2\sqrt{2}}\right)}{\sqrt{2}\pi}\right)^{d/2} \exp\left(-\frac{1}{\sqrt{2}}m\Omega \tanh\left(\frac{\beta\Omega}{2\sqrt{2}}\right)\mathbf{r}^{2}\right). \quad (5.49)$$

These quantities are now plotted alongside the density and pair correlation functions in Figure 5.4. For the density an exact agreement is seen which confirms that the single-particle correlation functions lose all their bosonic properties. For the pair correlation function at large distances an exact agreement is found, but at small distances the pair correlation function exhibits a sharp kink which only disappears in the true $W \to \infty$ limit. Therefore we conclude that even when the bosons acquire distinguishable labels, the bosonic properties remain robustly hidden at short distances in the pair correlation functions.

5.5 Conclusion

In this chapter we derived the one particle reduced density matrix, the density, and two-point correlation function for a general class of quadratic bosonic systems with retarded interactions in the canonical ensemble. As the bosons obtain an effective memory in this description, the commonly used composition properties of path integral propagators no longer hold, and a more general approach to compute the contribution of the permutation cycles is presented.

This formalism is then applied to a model of an open quantum system of



FIGURE 5.5: A depiction of the asymptotic limit of the model. When W is comparable to the trapping frequency Ω , the bosons can condense, largely remaining indistinguishable (a). When W is increased the particles are glued together and the bosons effectively acquire a distinguishable label (b). Finally note that this picture is less accurate for two-point correlations, even with the distinguishable labels the bosonic nature is retained in the pair-correlation function at short distances (c).

identical oscillators where some external environment is modeled by the memory effects of fictitious masses. We show how as the coupling strength with the environment is increased in the case of distinguishable particles entanglement with the environment results in a highly mixed state, whereas the bosonic case retains its macroscopic occupation of the ground state up to far stronger coupling strengths. This gives rise to uniquely bosonic non-monotonic behavior of the particle density as a function of the coupling strength, where at an intermediate coupling the bosons experience maximal trapping strength. In the context of the density and pair correlation function the strong coupling limit is discussed, where we show how at sufficiently strong coupling strength even at zero temperature the bosons become distinguishable, while retaining a trace of the bosonic statistics in the short-range part of the pair correlation function.

The presented results open up the semi-analytic treatment of an entirely new class of action functionals for a finite number of identical particles in the pathintegral formalism. Retarded interactions have already proven to be a powerful method in variational models for certain types of systems. With the present results, all the prerequisites to formulate a general variational model for identical particles are obtained, which will be discussed in more detail in the next chapter.

CHAPTER 6

Ground state properties of many polarons

In this final chapter of the thesis, we will proceed with what we set out to do in the introductory parts of Chapter 4 and investigate the many polaron ground state properties in a beyond mean field approach. This requires a synthesis of various results and techniques from the previous chapters. As we have seen in Chapter 3, methods relying on the Bogoliubov transformation appear to suffer from an instability on the attractive branch and for this reason mainly the repulsive branch will be studied.

In Sec. 6.1 we discuss the applicability of the Fröhlich and extended Fröhlich models for many polarons and argue that most of the techniques used for a single impurity can be used for multiple impurities as well. In Sec. 6.2, we show that the identical particle properties of the impurities become irrelevant for bosons at zero temperature what concerns the variational minimization. This provides motivation to proceed and study distinguishable impurities in Sec. 6.3. We study the ground state properties of the Fröhlich and extended Fröhlich models in Sec. 6.4 and Sec. 6.5.

6.1 Many particle extensions

6.1.1 The variational approach for identical particles

At the heart of the variational path integral approach lies the Jensen-Feynman inequality:

$$F \le F_0 + \frac{1}{\hbar\beta} \left\langle \mathcal{S}_{\text{eff}} - \mathcal{S}_0 \right\rangle, \tag{6.1}$$

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which allows one to obtain a variational upper bound to the free energy F of some difficult effective action S_{eff} through a simpler model action S_0 . For a single particle it is well known that as long as both action functionals are real the application of the inequality is justified. Indeed, as has been extensively discussed in Chapter 2, for a single impurity this approach can be successfully used to tackle the single polaron in the Bogoliubov-Fröhlich Hamiltonian if a sufficiently general S_0 is chosen. However, the validity of the inequality is not always guaranteed in more exotic circumstances. For example, in the presence of a magnetic field the action functionals contain imaginary contributions and depending on the form of the trial action, corrections beyond the inequality (6.1) might be required [117].

The question that concerns us going forward is whether or not the inequality of the form (6.1) can be used for multiple particles. In case of distinguishable particles in d dimensions, the answer can be easily obtained by noticing that in this case the many body path integral is merely a standard particle path integral in dN dimensions with the coordinates $(x_1, y_1, ..., x_2, y_2, ..., x_N, y_N, ...)$ for which the inequality is valid. However, for identical particles the end points of the path integral for the partition function have to be permuted:

$$\mathcal{Z}(N) = \frac{1}{N!} \sum_{P} \left(\xi\right)^{P} \int d\overline{\mathbf{r}} \int_{\overline{\mathbf{r}},0}^{P[\overline{\mathbf{r}}],\beta} \mathcal{D}\overline{\mathbf{r}}' \ e^{-S^{(N)}[\overline{\mathbf{r}}',x,y,\overline{\kappa}]},\tag{6.2}$$

where for fermions $\xi = -1$ and the terms gain an additional minus sign in every odd permutation, and for bosons $\xi = 1$ such that all terms yield a positive contribution. The question as to whether or not the Jensen-Feynman inequality can be applied to (6.2) has been discussed by J. T. Devreese in [118]. In summary, this work contains a simple demonstration of how for *fermions* the sign alternation in (6.2) forms a significant problem in the application of the inequality. It has been shown by Lemmens, Brosens and Devreese that the sign problem can be cured by representing the path integrals in terms of diffusive processes and that the variational inequality can be applied to fermions only on the condition of placing several restrictions upon the trial action S_0 [119]. However, for bosons the summation in (6.2) consists only of positive terms such that the previous concerns do not apply¹. We can directly quote [118]:

"Fermion systems (with parallel spins) form an important class of systems for which the Jensen-Feynman inequality is not directly ap-

¹I am grateful to S. N. Klimin for clarifying this point to me in correspondence.

plicable ... The reason for this is that the path integral for *fermions* with parallel spin, *if expressed in the full coordinate space*, is a superposition of path integrals with all possible permutations of the particle coordinates, with negative signs for all odd permutations. For *bosons*, no negative signs result from the permutations, and the application of the Jensen-Feynman inequality presents no problems"

- J. T. Devreese in [118]

Rigorously proving the Jensen-Feynman inequality for bosons is beyond the scope of the current chapter, and hence we proceed relying on the conclusions in the aforementioned studies that the inequality (6.1) can be safely used for bosons for any general model action functional S_0 . From the previous discussion it also follows that without making any additional restrictions the completely general action functional considered in Chapters 4 and 5 can be variationally applied to bosonic impurities as is the case in the Aarhus experiment [23]. For fermions in the JILA experiment [19] further restrictions on S_0 have to be placed.

6.1.2 The effective action for multiple particles

In expression (1.21) of Chapter 1 we have introduced the Bogoliubov-Fröhlich model described by

$$\hat{H}_F = \sum_{\mathbf{j}}^{N_I} \frac{\hat{\mathbf{p}}_j^2}{2m} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{g_{ib}\sqrt{N_0}}{V} \sum_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{-\mathbf{k}}^{\dagger} \right), \qquad (6.3)$$

where multiple impurities are accounted for in the density operator:

$$\hat{\rho}_{\mathbf{k}} = \sum_{j=1}^{N_I} e^{i\mathbf{k}\cdot\hat{\mathbf{r}}_j}.$$
(6.4)

It is clear that the function $\hat{\rho}_{\mathbf{k}}$ is unaffected by integrating out the phonons in (6.3) and hence the effective action for the Bogoliubov-Fröhlich model remains exactly the same as used for a single impurity:

$$\mathcal{S}_{\text{eff}}^{(\text{F})} = \int_0^{\hbar\beta} \frac{m\dot{\mathbf{r}}^2}{2} dt - \frac{1}{V} \sum_{\mathbf{k}} \frac{g_{ib}^2 n_0}{2\hbar} V_{\mathbf{k}}^2 \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma \mathcal{G}_{\mathbf{k}} \left(\tau - \sigma\right) \rho_{\mathbf{k}}(\tau) \rho_{\mathbf{k}}^*(\sigma), \quad (6.5)$$

with the emphasis that now the many-impurity density (6.4) is to be used.

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For the extended Fröhlich model

$$\hat{H}_{EF} = \sum_{\mathbf{j}}^{N_I} \frac{\hat{\mathbf{p}}_j^2}{2m} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{g_{ib}\sqrt{N_0}}{V} \sum_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{-\mathbf{k}}^{\dagger} \right) + \frac{g_{ib}}{V} \sum_{\mathbf{s}\neq\mathbf{0}} \sum_{\mathbf{k}\neq\mathbf{0}} \hat{\rho}_{\mathbf{k}-\mathbf{s}} W_{\mathbf{k},\mathbf{s}}^{(1)} \hat{\alpha}_{\mathbf{s}}^{\dagger} \hat{\alpha}_{\mathbf{k}} + \frac{1}{2} \frac{g_{ib}}{V} \sum_{\mathbf{s}\neq\mathbf{0}} \sum_{\mathbf{k}\neq\mathbf{0}} \hat{\rho}_{\mathbf{k}-\mathbf{s}} W_{\mathbf{k},\mathbf{s}}^{(2)} \left(\hat{\alpha}_{\mathbf{s}}^{\dagger} \hat{\alpha}_{-\mathbf{k}}^{\dagger} + \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{-\mathbf{s}} \right)$$

$$(6.6)$$

broadly the same argument holds, but a few details have to be addressed first. Note that the extended Fröhlich terms in (6.6) contain the impurity density in the following form: $\hat{\rho}_{\mathbf{k}-\mathbf{s}}$. In the analysis of a single impurity in Chapter 3, for convenience this expression has been occasionally split as $\hat{\rho}_{\mathbf{k}}\hat{\rho}_{\mathbf{s}}^*$, which is of course not valid for multiple impurities. Fortunately, in the set up of the derivation expressed in (3.11) this simplification is not made and hence the general strategy can equivalently be applied to the many particle case. Relying on the same approximations that were argued in Chapter 3, the effective action for many particles can still be written as:

$$\mathcal{S}_{\text{eff}} = \mathcal{S}_{\text{eff}}^F - \hbar \sum_{n=1}^{\infty} (-1)^n g_{ib}^n O_n.$$
(6.7)

However, for a single polaron, to write down the expression in (3.27):

$$O_{n}^{(\text{sp})} = \frac{g_{ib}^{2}n_{0}}{\hbar \left(2V\hbar\right)^{n+1}} \int_{0}^{\hbar\beta} d\tau_{1}...\int_{0}^{\hbar\beta} d\tau_{n+2} \times \sum_{\mathbf{k}_{1},...,\mathbf{k}_{n+1}} \left(\prod_{j=1}^{n+1} V_{\mathbf{k}_{j}}^{2}\mathcal{G}_{\mathbf{k}_{j}}\left(\tau_{j+1}-\tau_{j}\right)\rho_{\mathbf{k}_{j}}(\tau_{j})^{*}\rho_{\mathbf{k}_{j}}(\tau_{j+1})\right), \qquad (6.8)$$

we have made the aforementioned factorization $\rho_{\mathbf{k}-\mathbf{s}} = \rho_{\mathbf{k}}\rho_{\mathbf{s}}^*$ for the singly impurity. If the factorization is not used to simplify the scattering terms in Chapter 3, for multiple polarons the appropriate expression reads:

$$O_{n} = \frac{g_{ib}^{2} n_{0}}{\hbar \left(2V\hbar\right)^{n+1}} \int_{0}^{\hbar\beta} d\tau_{1} \dots \int_{0}^{\hbar\beta} d\tau_{n+2} \sum_{\mathbf{k}_{1},\dots,\mathbf{k}_{n+1}} \prod_{j=1}^{n+1} \left(V_{\mathbf{k}_{j}}^{2} \mathcal{G}_{\mathbf{k}_{j}}\left(\tau_{j+1}-\tau_{j}\right)\right) \\ \times \rho_{\mathbf{k}_{1}}^{*}(\tau_{1}) \left(\prod_{j=1}^{n} \rho_{\mathbf{k}_{j}-\mathbf{k}_{j+1}}(\tau_{j+1})\right) \rho_{\mathbf{k}_{n+1}}(\tau_{n+2}),$$
(6.9)

which exactly agrees with the form in [91], where the factorization for a single

impurity was not implemented in the notation.

With this general form for O_n we run into an issue. It is not clear how the random phase approximation that has been devised for a single impurity and *a posteriori* justified in Chapter 3 generalizes to multiple impurities. This approximation was used to compute $\langle O_n \rangle$ with respect to the model action – a necessary step for the variational application. To explore this question for multiple impurities, first note that in the expectation value of O_n only the product of impurity densities in (6.9) will be of importance and hence the question of interest is how to compute:

$$W_n = \left\langle \rho_{\mathbf{k}_1}^*(\tau_1) \left(\prod_{j=1}^n \rho_{\mathbf{k}_j - \mathbf{k}_{j+1}}(\tau_{j+1}) \right) \rho_{\mathbf{k}_{n+1}}(\tau_{n+2}) \right\rangle.$$
(6.10)

Even with respect to the most trivial model system of free particles, the integral in (6.9) cannot be computed for arbitrary n. This should not come as a surprise, the series in (6.7) contains arbitrarily large powers of the coupling parameter g_{ib} , and hence knowing how to compute the expectation value $\langle S_{\text{eff}} \rangle$ with respect to free particles would be equivalent to knowing how to exactly compute contributions of Feynman diagrams of any order in the full polaron action. To proceed we will justify a random phase like approximation similar to the one proposed in Chapter 3, now applied to multiple particles.

First, consider the expectation value arising from the O_1 term:

$$W_{1} = \left\langle \rho_{\mathbf{k}_{1}}^{*}(\tau_{1})\rho_{\mathbf{k}_{1}-\mathbf{k}_{2}}(\tau_{2})\rho_{\mathbf{k}_{2}}(\tau_{3})\right\rangle$$

= $\sum_{i_{2}}\left\langle \sum_{i_{1},i_{3}}\exp\left(i\mathbf{k}_{1}\cdot\left[\mathbf{r}_{\mathbf{i}_{2}}(\tau_{2})-\mathbf{r}_{\mathbf{i}_{1}}(\tau_{1})\right]\right)\exp\left(i\mathbf{k}_{2}\cdot\left[\mathbf{r}_{\mathbf{i}_{3}}(\tau_{3})-\mathbf{r}_{\mathbf{i}_{2}}(\tau_{2})\right]\right)\right\rangle.$
(6.11)

A similar question as to how to approximate many-impurity correlations has been encountered in a mean field study of this problem in [59]. The authors propose to neglect the third central moment of W_1 with the operators expanded around their mean field value $\rho - \langle \rho \rangle$ in the following way:

$$\sum_{i_1,i_2,i_3} \left\langle \left(e^{i\mathbf{k_1} \cdot \left(\mathbf{r_{i_2}}(\tau_2) - \mathbf{r_{i_1}}(\tau_1) \right)} - \frac{1}{N_I^2} \sum_{i_1,i_2} \left\langle e^{i\mathbf{k_1} \cdot \left(\mathbf{r_{i_2}}(\tau_2) - \mathbf{r_{i_1}}(\tau_1) \right)} \right\rangle \right)$$

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$$\left(e^{i\mathbf{k}_{2}\cdot\left(\mathbf{r}_{\mathbf{i}_{3}}(\tau_{3})-\mathbf{r}_{\mathbf{i}_{2}}(\tau_{2})\right)}-\frac{1}{N_{I}^{2}}\sum_{i_{1},i_{2}}\left\langle e^{i\mathbf{k}_{2}\cdot\left(\mathbf{r}_{\mathbf{i}_{3}}(\tau_{3})-\mathbf{r}_{\mathbf{i}_{2}}(\tau_{2})\right)}\right\rangle\right)\right\rangle \approx 0,\quad(6.12)$$

from which follows:

$$\sum_{i_1,i_2,i_3} \left\langle e^{i\mathbf{k_1} \cdot \left(\mathbf{r_{i_2}}(\tau_2) - \mathbf{r_{i_1}}(\tau_1)\right)} e^{i\mathbf{k_2} \cdot \left(\mathbf{r_{i_3}}(\tau_3) - \mathbf{r_{i_2}}(\tau_2)\right)} \right\rangle$$
$$\approx \frac{1}{N_I} \sum_{i_1,i_2} \left\langle e^{i\mathbf{k_1} \cdot \left(\mathbf{r_{i_2}}(\tau_2) - \mathbf{r_{i_1}}(\tau_1)\right)} \right\rangle \sum_{i_2,i_3} \left\langle e^{i\mathbf{k_2} \cdot \left(\mathbf{r_{i_3}}(\tau_3) - \mathbf{r_{i_2}}(\tau_2)\right)} \right\rangle. \tag{6.13}$$

This directly implies the following approximation for the expectation value of interest:

$$W_1 \approx \frac{1}{N_I} \left\langle \rho_{\mathbf{k}_1}^*(\tau_1) \rho_{\mathbf{k}_1}(\tau_2) \right\rangle \left\langle \rho_{\mathbf{k}_2}^*(\tau_2) \rho_{\mathbf{k}_2}(\tau_3) \right\rangle.$$
(6.14)

Therefore, we precisely retrieve the random phase approximation made in Chapter 3, now for multiple impurities. Similar arguments can be constructed for the general case to find:

$$W_{n} \approx \frac{1}{N_{I}^{n}} \left\langle \rho_{\mathbf{k}_{1}}^{*}(\tau_{1}) \rho_{\mathbf{k}_{1}}(\tau_{2}) \right\rangle \left\langle \rho_{\mathbf{k}_{2}}^{*}(\tau_{2}) \rho_{\mathbf{k}_{2}}(\tau_{3}) \right\rangle \dots \left\langle \rho_{\mathbf{k}_{n+1}}^{*}(\tau_{n+1}) \rho_{\mathbf{k}_{n+1}}(\tau_{n+2}) \right\rangle.$$
(6.15)

It is easy to see that the normalization factor N_I^n in front of the right hand side has to be there. For example, consider the case where all $\mathbf{k}_j = 0$. The left hand side of (6.15) then yields N_I^{n+2} . The product of expectation values on the right hand side yields $N_I^{2(n+1)}$ from which the necessity of the normalization factor can be readily understood. We can now proceed to apply this approximation to compute the effective action.

It is not difficult to show that for any function f(u) that obeys β periodicity such that $f(\beta - u) = f(u)$:

$$\int_{0}^{\beta} d\tau_{1}...d\tau_{n+2}f(\tau_{1}-\tau_{2})...f(\tau_{n+1}-\tau_{n+2}) = \beta 2^{n+1} \left(\int_{0}^{\beta/2} f(u)\right)^{n+1}$$
$$= \beta 2^{n+1} \left(\frac{1}{2\beta} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\sigma f(\tau-\sigma)\right)^{n+1}$$
(6.16)

If we also assume that the expectation value $\langle \rho_{\mathbf{k}}(\tau) \rho_{\mathbf{k}}^*(\sigma) \rangle$ only depends on the time difference and is also β -periodic, we obtain our previous expression for the random phase approximate effective action (3.36), now also accounting for the
normalizing factor:

$$\left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle_{0} = g_{ib} n_{0} \hbar \beta \sum_{n=1}^{\infty} \frac{1}{N_{I}^{n-1}} \left(-\frac{g_{ib}}{\hbar V} \frac{1}{2\beta} \sum_{\mathbf{k}} V_{\mathbf{k}}^{2} \int_{0}^{\hbar \beta} d\tau \int_{0}^{\hbar \beta} d\sigma \mathcal{G}_{\mathbf{k}} \left(\tau - \sigma\right) \left\langle \rho_{\mathbf{k}}(\tau) \rho_{\mathbf{k}}^{*}(\sigma) \right\rangle \right)^{n},$$

$$\tag{6.17}$$

where we use the tilde to indicate the subtraction of the kinetic energy as in Chapter 2. Remember that for N_I impurities the mean-field impurity-condensate shift $N_I g_{ib} n_0$ gets multiplied by N_I as well, such that:

$$\frac{1}{\hbar\beta} \left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle_{0} + N_{I} g_{ib} n_{0} \\
= N_{I} g_{ib} n_{0} \sum_{n=0}^{\infty} \left(-\frac{g_{ib}}{\hbar V} \frac{1}{2\beta} \sum_{\mathbf{k}} V_{\mathbf{k}}^{2} \int_{0}^{\hbar\beta} d\tau \int_{0}^{\hbar\beta} d\sigma \mathcal{G}_{\mathbf{k}} \left(\tau - \sigma\right) \left\langle \rho_{\mathbf{k}}(\tau) \rho_{\mathbf{k}}^{*}(\sigma) \right\rangle \right)^{n}.$$
(6.18)

If Lippmann-Schwinger renormalization is now performed by substituting the full expression for $g(\Lambda)$ as given in (3.38), we obtain the following resummation of the effective action:

$$\frac{1}{\hbar\beta} \left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle_0 = \frac{g_{ib} n_0 N_I}{1 + g_{ib} \Gamma[x, y]} - N_I g_{ib} n_0, \tag{6.19}$$

with from this point onward, g_{ib} being just the lowest order expression at $\Lambda = 0$. This result is of course nothing else than the energy term with the resonance shift obtained in the last term of (3.39), where:

$$\Gamma[x,y] = \frac{1}{2\hbar\beta V} \sum_{\mathbf{k}} V_{\mathbf{k}}^2 \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma \mathcal{G}_{\mathbf{k}} \left(\tau - \sigma\right) \frac{1}{N_I} \left\langle \rho_{\mathbf{k}}(\tau) \rho_{\mathbf{k}}^*(\sigma) \right\rangle - \frac{1}{V} \sum_{\mathbf{k}} \frac{2\mu}{\hbar^2 k^2},$$
(6.20)

and the brackets indicate that Γ can still be a function(al) of variational parameters. This allows us now to write the variational free energy for many polarons in the extended Fröhlich model as:

$$F_{v}^{(\text{EF})}[x,y] = F_{0}[x,y] - \frac{1}{\hbar\beta} \left\langle S_{0} \right\rangle + \frac{g_{ib}n_{0}N_{I}}{1 + g_{ib}\Gamma[x,y]} - N_{I}g_{ib}n_{0}, \qquad (6.21)$$

and the result for the Fröhlich model is found by expanding the expression up to

lowest order in Γ :

$$F_{v}^{(\mathrm{F})}[x,y] = F_{0}[x,y] - \frac{1}{\hbar\beta} \langle \mathcal{S}_{0} \rangle - g_{ib}^{2} n_{0} N_{I} \Gamma[x,y].$$
(6.22)

While expression (6.22) is true regardless of the model action, in the previous derivation of (6.21) we have assumed that $\langle \rho(\tau)\rho(\sigma)^* \rangle$ only depends on the time difference $\tau - \sigma$ and is in addition β -periodic to use the property (6.16).

6.2 General model system for bosons at zero temperature

In this section we will address an important point regarding the general action functional formalism for bosons and illustrate how the variational model behaves at zero temperature. As argued before in the previous section, to use $S_0[x, y]$ as a variational model for bosons, no restrictions are required aside from the ones discussed in Chapters 4 and 5. Therefore, in principle the most general form of S_0 can be used as a variational model for a system of bosons without any issue (for $\hbar = 1$):

$$S^{(N)}[x,y] = \frac{m}{2} \sum_{i}^{N} \int_{0}^{\beta} \dot{\mathbf{r}}_{i}(\tau)^{2} d\tau + \frac{m}{2} \sum_{i}^{N} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\sigma x(\tau-\sigma) \mathbf{r}_{i}(\tau) \cdot \mathbf{r}_{i}(\sigma) + \frac{m}{2N} \sum_{i,j}^{N} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\sigma \left[y(\tau-\sigma) - x(\tau-\sigma) \right] \mathbf{r}_{i}(\tau) \cdot \mathbf{r}_{j}(\sigma).$$
(6.23)

However, not all realizations of S_0 have a transparent physical interpretation. In particular when the memory kernel $x(\tau - \sigma) \neq 0$, a subtle issue can be observed already on a qualitative level. In this case, a particle with coordinate \mathbf{r}_i interacts with itself through a different memory kernel than with another particle with coordinate \mathbf{r}_j . For example, consider the case where $x \neq 0$ and x = y, such that each boson interacts only with itself and previous times, but is not affected by any other boson. The natural question arises, what kind of physical system is capable of creating an instance where identical particles are discerning between one another in the past?

It therefore seems to be the case that while any S_0 can be used as a trial function, not every S_0 of the form (6.23) actually corresponds to a realistic system of bosonic particles. While this does not form a fundamental problem for the purposes of our applications, some caution is required to physically interpret such realizations of S_0 . Indeed, precisely a system of this type was considered in our example applications of Chapter 4 and Chapter 5. Although the results are physically sound and the appropriate limiting cases are retrieved, one issue that has not been addressed is already present in the Lagrangian (4.26) of Chapter 4. By coupling the bosons to distinguishable particles in this way, we are making the assumption that the distinguishable particles are somehow capable of discerning the bosons, which is of course an unnatural coupling for realistic physical systems. This in turn gives raise to the type of memory effects in the action functional described in the previous paragraph. Therefore, we emphasize that thermodynamic quantities or correlation functions corresponding to the most general form of the action functional (6.23) are to be interpreted strictly in the context of the behavior of variational models. This means that the free energy and the correlation functions are to be interpreted as the quantities that respectively correspond to F_0 and to the expectation values $\langle ... \rangle$ that are used in the inequality (6.1).

Having addressed this important caveat we now proceed to discuss the behavior of the model system at zero temperature. We start by investigating the central quantity that appears throughout the derivations in Chapter 4 and Chapter 5:

$$\Delta_x A_x - 1 = \frac{4}{\beta^2} \sum_{n = -\infty}^{\infty} \frac{1}{\nu_n^2 + \tilde{x}_n} \sum_{n' = -\infty}^{\infty} \frac{\tilde{x}_{n'}}{\nu_{n'}^2 + \tilde{x}_{n'}} - 1, \qquad (6.24)$$

where for convenience of notation we have redefined $\tilde{x}_n = \beta x_n$. Let us now discern two possible cases. The first option is that the memory kernel x_n could be constant in Fourier space which corresponds to a simple harmonic trap $\tilde{x}_n = \omega^2$. In this case the summations in (6.24) are readily performed to find:

$$\Delta_x A_x - 1 = \coth\left(\frac{\beta\omega}{2}\right) - 1. \tag{6.25}$$

In the limit of zero temperature $\beta \to \infty$ this expression goes to zero and hence some care should be taken since (6.25) appears at various places in our framework. We have checked that in this case exactly at T = 0, all quantities of further interest in this chapter such as the partition function or correlation functions reduce to the distinguishable particle case and lose their bosonic properties. This should not come as a surprise – from an energy point of view, at zero temperature both bosons and distinguishable particles will simply completely fill up the non-degenerate ground state and hence produce identical thermodynamic properties.

Although this seems quite obvious for the case of harmonically trapped particles, let us be more careful and check it in the presence of a non-trivial kernel $\tilde{x}_n \neq \text{cst.}$ In this case expression (6.25) does not necessarily go to zero as $\beta \to \infty$, which can also be easily checked from expressions (4.30) and (4.31) for our fictitious model in Chapter 4. At zero temperature, the recurrence part of the partition function therefore remains finite:

$$\mathbb{Z}(N) = \frac{1}{N} \sum_{k=0}^{N-1} \mathbb{Z}(k) \left| 2 \sinh\left[\frac{(N-k)}{2} \operatorname{arccosh}\left(\frac{A_x \Delta_x + 1}{A_x \Delta_x - 1}\right)\right] \right|^{-d}.$$
 (6.26)

It follows that the last two terms drop out from the free energy of the model action:

$$F_{0} = \frac{3(N-1)}{\beta} \sum_{k=1}^{\infty} \log\left(1 + \frac{\tilde{x}_{k}}{\nu_{k}^{2}}\right) + \frac{3}{\beta} \sum_{k=1}^{\infty} \log\left(1 + \frac{\tilde{y}_{k}}{\nu_{k}^{2}}\right) + \frac{3N}{2\beta} \log\left(\frac{1}{4}\beta \tilde{x}_{0}(\Delta_{x}A_{x}-1)\right) - \frac{1}{\beta} \log\left(\mathbb{Z}_{N}\right).$$
(6.27)

which yields at zero temperature:

$$F_0 = \frac{3(N-1)}{2\pi} \int_0^\infty d\nu \log\left(1 + \frac{\tilde{x}(\nu)}{\nu^2}\right) + \frac{3}{2\pi} \int_0^\infty d\nu \log\left(1 + \frac{\tilde{y}(\nu)}{\nu^2}\right).$$
(6.28)

This is precisely the free energy for distinguishable particles.

The next part of the inequality is the expectation value of the model action with respect to itself $\langle \tilde{S}_0 \rangle$. This identity is most easily computed by introducing a scaling parameter λ to the interaction parts of S_0 such that $x \to \lambda x$ and $y \to \lambda x$ to obtain the dependence of the free energy $F_0(\lambda)$ on the scaling parameter. The expectation value is then computed as:

$$\frac{1}{\beta} \left\langle \tilde{\mathcal{S}}_{0} \right\rangle = \beta \partial_{\lambda} F_{0}(\lambda)|_{\lambda=1} = \frac{3(N-1)}{\beta} \sum_{k=1} \frac{\tilde{x}_{k}}{\nu_{k}^{2} + \tilde{x}_{k}} + \frac{3}{\beta} \sum_{k=1} \frac{\tilde{y}_{k}}{\nu_{k}^{2} + \tilde{y}_{k}} \\
+ \frac{3N}{2\beta} \left[1 + \frac{\partial_{\lambda} A_{\lambda x} \Delta_{\lambda x}|_{\lambda=1}}{A_{x} \Delta_{x} - 1} \right] - \frac{1}{\beta \mathbb{Z}_{N}} \partial_{\lambda} \mathbb{Z}_{N}(\lambda)|_{\lambda=1}.$$
(6.29)

Given that both the partition function and $A_x \Delta_x$ are finite at zero temperature for any λx , unless the derivatives ∂_{λ} diverge the last two terms drop out and we once again obtain the zero-temperature expression of distinguishable particles:

$$\left\langle \tilde{\mathcal{S}}_{0} \right\rangle = \frac{3(N-1)}{2\pi} \int_{0}^{\infty} d\nu \frac{\tilde{x}(\nu)}{\nu^{2} + \tilde{x}(\nu)} + \frac{3}{2\pi} \int_{0}^{\infty} d\nu \frac{\tilde{y}(\nu)}{\nu^{2} + \tilde{y}(\nu)}.$$
 (6.30)

It turns out that in the Bogoliubov-Fröhlich model at zero temperature the expectation value of the effective action $\langle S_{\text{eff}} \rangle$ can also be computed as if the particles are distinguishable. The argument is slightly technical and an overview is relegated to Appendix J. With this result, together with (6.28) and (6.30), we conclude that at zero temperature for bosonic impurities identical particle statistics can be neglected when it comes to an application of our variational framework. Although we only prove it within the Bogoliubov-Fröhlich model, it is reasonable to assume this to also be true for more general polaron models and hence we will use this result for the extended Fröhlich model as well. Since for distinguishable particles, the expectation value $\mathcal{F}_{\mathbf{k}}(u)$ only depends on the time difference and is β -periodic as well, in this case the result (6.21) can be used for the extended Fröhlich model.

6.3 Distinguishable polarons

Relying on the previous discussion, we proceed to study the case of distinguishable impurities which we have identified to be equivalent to bosonic impurities in the zero temperature limit of the general memory variational framework. We note that even this distinguishable particle limit forms a non-trivial extension of the results in Chapter 2 and has thus far not been performed in the literature with general memory kernels. To be able to make a clear comparison with the results of Chapter 2 further on, from this point on we redefine the notation $\tilde{x}_n \to x_n$ to avoid having to carry the tilde everywhere. As shown in Appendix J, the correlation functions for distinguishable particles within the general memory kernel formalism are given by:

$$\mathcal{F}_{\mathbf{k}}(\tau-\sigma) = \langle \rho_{\mathbf{k}}(\tau_1)\rho_{\mathbf{k}}^*(\sigma) \rangle = N\mathcal{F}_{\mathbf{k}}^{(1)}(\tau-\sigma) + N(N-1)\mathcal{F}_{\mathbf{k}}^{(2)}(\tau-\sigma), \quad (6.31)$$

where:

$$\mathcal{F}_{\mathbf{k}}^{(1)}(\tau - \sigma) = \exp\left(-\frac{k^2}{4m}\varphi(\tau - \sigma)\right),\tag{6.32}$$

$$\mathcal{F}_{\mathbf{k}}^{(2)}(\tau - \sigma) = \exp\left(-\frac{k^2}{4m}\xi(\tau - \sigma)\right).$$
(6.33)

The exponents are defined as:

$$\varphi(\tau - \sigma) = \frac{1}{N} \{ (N - 1) \left[D_x(0) - D_x(\tau - \sigma) \right] + D_y(0) - D_y(\tau - \sigma) \}, \quad (6.34)$$

$$\xi(\tau - \sigma) = \frac{1}{N} \left[(N - 1)D_x + D_y + D_x(\tau - \sigma) - D_y(\tau - \sigma) \right], \tag{6.35}$$

using a shorthand notation $D_x = D_x(0)$, where:

$$D_x(u) = \frac{4}{\beta} \sum_{n=-\infty}^{\infty} \frac{e^{i\nu_n u}}{\nu_n^2 + x_n}.$$
 (6.36)

These expressions have the same symmetry as in the case of a single impurity, which allows us to write the previously defined $\Gamma[x, y]$ in (6.20) as:

$$\Gamma[x,y] = \frac{1}{V} \sum_{\mathbf{k}} V_{\mathbf{k}}^2 \int_0^{\hbar\beta/2} du \mathcal{G}_{\mathbf{k}}(u) \left[\mathcal{F}_{\mathbf{k}}^{(1)}(u) + (N_I - 1) \mathcal{F}_{\mathbf{k}}^{(2)}(u) \right] - \frac{1}{V} \sum_{\mathbf{k}} \frac{2\mu}{\hbar^2 k^2}.$$
 (6.37)

After substituting F_0 and $\langle S_0 \rangle$ into the variational free energies of the Fröhlich (6.22) and extended Fröhlich models (6.21), respectively, we obtain:

$$F_{v}^{(\mathrm{F}/\mathrm{EF})}[x,y] = \frac{3(N-1)}{\beta} \sum_{k=1}^{\infty} \log\left(1 + \frac{x_{k}}{\nu_{k}^{2}}\right) + \frac{3}{\beta} \sum_{k=1}^{\infty} \log\left(1 + \frac{y_{k}}{\nu_{k}^{2}}\right) - \frac{3(N-1)}{\beta} \sum_{k=1} \frac{x_{k}}{\nu_{k}^{2} + x_{k}} - \frac{3}{\beta} \sum_{k=1} \frac{y_{k}}{\nu_{k}^{2} + y_{k}} - \frac{g_{ib}^{2} n_{0} N_{I} \Gamma[x,y]}{1 + g_{ib} \Gamma[x,y]^{(\mathrm{EF})}}.$$
(6.38)

where the $\sim g_{ib}$ correction in the denominator of the last term is only to be accounted for in the extended Fröhlich model and neglected within the Fröhlich model.

It is now a straightforward minimization problem to obtain the equations for the variational minimum $\nabla_{x,y}F_v = 0$ by deriving $\partial_{x_n}F_v = \partial_{y_n}F_v = 0$ and obtaining:

$$x(\nu) = \frac{8}{3\pi^2} \frac{g_{ib}^2 n_0}{8m\hbar} \left[J_1 + (N-1)J_2 - \Gamma_1(\nu) + \Gamma_2(\nu) \right], \tag{6.39}$$

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$$y(\nu) = \frac{8}{3\pi^2} \frac{g_{ib}^2 n_0}{8m\hbar} \left[J_1 + (N-1)J_2 - \Gamma_1(\nu) - (N-1)\Gamma_2(\nu) \right], \tag{6.40}$$

where the terms on the RHS are functionals of x and y themselves:

$$J_1 = \int dk k^4 V_k^2 \int_0^{\frac{\hbar\beta}{2}} du \mathcal{G}_{\mathbf{k}}(u) \exp\left(-\frac{k^2}{4m}\varphi\right), \qquad (6.41)$$

$$J_2 = \int dk k^4 V_k^2 \int_0^{\frac{\hbar\beta}{2}} du \mathcal{G}_{\mathbf{k}}(u) \exp\left(-\frac{k^2}{4m}\xi\right),\tag{6.42}$$

$$\Gamma_1(\nu) = \int dk k^4 V_k^2 \int_0^{\frac{h\beta}{2}} du \mathcal{G}_{\mathbf{k}}(u) \exp\left(-\frac{k^2}{4m}\varphi\right) \cos(\nu u), \qquad (6.43)$$

$$\Gamma_2(\nu) = \int dk k^4 V_k^2 \int_0^{\frac{\hbar\beta}{2}} du \mathcal{G}_{\mathbf{k}}(u) \exp\left(-\frac{k^2}{4m}\xi\right) \cos(\nu u).$$
(6.44)

This approach forms a direct extension of the treatment of the single polaron in Chapter 2 to multiple impurities, however to make a direct comparison some care should be taken. In Chapter 2 we have implicitly assumed that the memory kernel goes to zero in frequency space, i.e. $x_0 = 0$, whereas starting from Chapter 4 we have been working under the assumption $x_0 \neq 0$ and $y_0 \neq 0$.

To confirm that the limit $x_0 \to 0$ is still correctly captured in this approach and yields no issues, let us try to retrieve the single polaron result in this formalism. To do so, we start by setting the memory kernels equal to one another $x_n = y_n$ such that the induced impurity interactions in (6.23) drop out. It follows that in this limit $\varphi(u) = D_x(0) - D_x(u)$ and $\xi(u) = D_x(0)$. For $x_0 \to 0$, we can clearly see that $D_x(0)$ as defined in (6.36) diverges, whereas this divergence cancels in $D_x(0) - D_x(u)$ for any u. This divergence of $\xi(u)$ has the effect of exponentially damping the second term $\mathcal{F}_{\mathbf{k}}^{(2)}(u)$ and removing it from the density correlation function (6.31). We can see that the remaining correlation $\mathcal{F}_{\mathbf{k}}^{(1)}$ is simply the single impurity result in (2.20) and the free energy (6.38) then corresponds to the variational energy of the single polaron (2.23) obtained in Chapter 2, now multiplied by N_I . Therefore, it appears that the restriction can be lifted while still retrieving the appropriate limits and hence we can omit the restriction $x_0 \neq 0$ in what follows.

Note that previously in our paper [111] we have made a comment regarding restricting $\Delta_x < \Delta_y$ for the purpose of stability conditions when performing the center of mass integral. However, this restriction is in fact too strict, and this center of mass integral could be performed later in the derivation similar to [107]

where this condition would no longer be required. From the discussion in [107] we can see that for *attractive* interparticle interactions, as will be shortly evidently observed here, we have no such restrictions and we only have to make sure that $\Delta_x > 0$ and $\Delta_y > 0$. Given that in what follows we always obtain positive $x(\nu)$ and $y(\nu)$ this condition is automatically satisfied.

Having addressed these points, we can proceed to solve equations (6.39) and (6.40) with a similar iterative method as presented in Chapter 2. After an initial guess for $\{x_n, y_n\}$ is substituted in the right hand side of (6.39) and (6.40), one obtains an improved suggestion for the memory kernels on the left hand side. This procedure is then iterated, where after each step the free energy (6.38) is evaluated and compared to the previous step until the difference drops below 1% which will be accepted as the final value. To represent the continuous memory kernels, we select a Gauss-Legendre quadrature on a logarithmically transformed $\nu = e^z - 1$ grid of 1000 points. Due to the smaller cutoff of $\Lambda \approx 190\xi^{-1}$ used further on we can use a smaller frequency cutoff $\nu_{\text{max}} = 10^6 \hbar/(m\xi^2)$.

We close the discussion of the energy minimization with one final word of caution. For multiple impurities, the variational landscape will always contain the non-interacting N_I polaron state as a possible local minimum. It is therefore now more important to be careful about whether the true minimum is reached. In what follows we observe that the non-trivial solution, where the polarons are strongly interacting, is most easily found either at large α or at large N_I . When making a plot as a function of α such as in Figure 6.1, it can therefore be useful to first find the interacting non-trivial solution at large α such that $x_n \neq y_n$, and then use this result as the initial guess for a smaller $\alpha - d\alpha$ to track this solution. At some sufficiently small critical value of α this solution appears to transition into N_I copies of the single polaron, indicating the absence of polaron binding in this regime.

One other interesting quantity that will turn out to be illustrative further on is the spatial distribution of the impurities. However, in the absence of an external harmonic trapping potential as considered in Chapter 5, our focus should lie on computing relative coordinates, rather than absolute density profiles themselves. It is well known that for a single polaron the spatial profile of the impurity is completely delocalized at any coupling strength. This can be easily seen from expression (2.12), from which follows that if the optimal memory kernel at small frequencies $\nu \to 0$ behaves as $x(\nu) \approx \nu^n$ with n > 1, which is indeed found to be the optimal solution for a single polaron, the expectation value $\langle \mathbf{r}^2 \rangle$ diverges. This should not come as a surprise – the polaron system has translational symmetry and hence only correlations between the impurity and the condensate become localized. For example, the polaron radius studied in (3.43), is technically defined as the relative coordinate between the impurity and the fictitious mass in Feynman's original system $\langle (\mathbf{r} - \mathbf{Q})^2 \rangle$ which is localized in contrast to $\langle \mathbf{r}^2 \rangle$. For this exact reason, when probing the spatial properties of the many polaron system, it is most convenient to study the correlations between \mathbf{r}_i and \mathbf{r}_j rather than the absolute density profiles themselves. For $i \neq j$ we define the average inter-impurity distance that will be used in the following section as:

$$R_{12} = \sqrt{\left\langle \left(\mathbf{r}_i - \mathbf{r}_j\right)^2 \right\rangle}.$$
(6.45)

If we remember that:

$$\mathcal{F}_{\mathbf{k}}^{(2)}(\tau,\sigma) = \left\langle e^{i\mathbf{k}[\mathbf{r}_{i}(\tau)-\mathbf{r}_{j}(\sigma)]} \right\rangle, \tag{6.46}$$

for an optimized memory kernel x_n we can obtain the average impurity separation at zero temperature as:

$$R_{12}^{2} = -\nabla_{\mathbf{k}}^{2} \mathcal{F}_{\mathbf{k}}^{(2)}(0,0) \Big|_{\mathbf{k}=0} = \frac{6}{4m} D_{x}(0) = \frac{6}{m\pi} \int_{0}^{\infty} d\nu \frac{1}{\nu^{2} + x(\nu)}.$$
 (6.47)

From this expression we can see that if $x(\nu) \to 0$ at small frequencies, the impurity correlations will be delocalized. As discussed before, this solution corresponds to the N_I noninteracting polaron state and hence this is to be expected. However, once non-trivial many polaron interactions start to become noticeable in the energy the optimal memory kernel will have $x(0) \neq 0$ and a finite value for (6.47) is obtained, indicating a localization of the impurity-impurity correlations.

We could go one step further and take a look at the two-point correlation density $g(\mathbf{r})$:

$$g(\mathbf{r}) = \frac{1}{N_I} \frac{1}{(2\pi)^3} \int \mathbf{dk} \left\langle \sum_{i \neq j} e^{i\mathbf{k} \cdot [\mathbf{r}_i(0) - \mathbf{r}_j(0)]} \right\rangle e^{-i\mathbf{k} \cdot \mathbf{r}}$$
$$= (N_I - 1) \left(\frac{m}{\pi D_x(0)}\right)^{3/2} \exp\left(-\frac{mr^2}{D_x(0)}\right). \tag{6.48}$$

This quantity represents the effective density profile as seen in the frame of one of the impurities, which allows one to avoid the aforementioned subtlety with

localization. We can indeed see from (6.48) that it is normalized to $N_I - 1$ and that $D_x(0)/m$ plays the role of the profile width as reflected in the radius (6.47).

6.4 Comparison between the Fröhlich and extended Fröhlich models for multiple impurities

In this section we will compare the ground state energy of the Fröhlich and the extended Fröhlich for multiple impurities in a BEC at zero temperature. As we have previously argued within our variational framework, bosonic impurities at zero temperature can be studied in the distinguishable particle approach of the last section. For this reason we are mainly interested using the system parameters of the Aarhus experiment [23], where bosonic ³⁹K impurities were immersed in a condensate of the same atoms in a different hyperfine state such that $m = m_b$. For further details of the experiment we refer the reader to the discussion in Chapter 1 or the papers accompanying the experiment [23, 46]. The cutoff value of the momentum integrals is chosen equal to the Van der Waals length of ³⁹K, which roughly corresponds to $\Lambda \approx 190\xi^{-1}$ [23, 70]. To obtain the zero-temperature result we use a large inverse temperature cutoff corresponding to $\beta = 200\hbar/(m\xi^2)$. Since the effect of Efimov physics and going beyond the Bogoliubov approximation has been argued to be important on the attractive branch [45] we will be focusing on the repulsive branch here. The boson-boson scattering length is tuned to $a_{bb} = 9a_0$ in the experiment and kept constant, and hence either $\alpha = a_{ib}^2/(a_{bb}\xi^2)$ or $(k_n a_{ib})^{-1}$ with $k_n = (6\pi^2 n_0)^{1/3}$ can both be unambiguously used as the interaction parameter between the impurity and condensate on the repulsive branch where $a_{ib} > 0$. In the experiment the impurities exhibit a weak direct attraction corresponding to roughly $a_{ii} = -20a_0$. Towards stronger coupling this value is far smaller than the scattering length with the condensate a_{ib} . Moreover, the induced interactions on the repulsive branch are attractive and any additional small attraction between the impurities themselves should not significantly change the conclusions. Therefore, we will be considering non-interacting impurities in what follows.

In Figure 6.1 we start by presenting a comparison between the ground state energy per polaron within the Fröhlich and extended Fröhlich models. With the mass ratio $m = m_b$, the impurity is significantly heavier here than in the previously considered case in Chapter 2. Hence, we can immediately observe that it takes stronger interaction strengths $\alpha \approx 6$ for the single-impurity polaronic energy to become negative, which is the point at which polaronic effects start to occur. This 6.4 - Comparison between the Fröhlich and extended Fröhlich models for multiple impurities



FIGURE 6.1: Polaronic energy per impurity within the Bogoliubov-Fröhlich model (a) and the extended Fröhlich model (b) for the system parameters of the Aarhus experiment [23], $m = m_b$ and $\Lambda \approx 190\xi^{-1}$ at zero temperature.



FIGURE 6.2: Polaronic energy per impurity within the Bogoliubov-Fröhlich model (solid circles) and the extended Fröhlich model (solid squares) as a function of the impurity number in the units of the Aarhus experiment at a fixed interaction strength $(a_{ib}k_n)^{-1} = 1.6$ or $\alpha = 2.386$. The energy is measured with respect to $\hbar^2 k_n^2/(2m)$ to use the same convention as [23]. The inset shows the extended model results op to $N_I = 500$.

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FIGURE 6.3: Polaronic energy per impurity within the Bogoliubov-Fröhlich model (solid circles) and the extended Fröhlich model (solid squares) as a function of the impurity number. The system parameters of Chapter 2 for a light impurity $m_b = 3.8m$ at moderately weak coupling $\alpha = 1$ are used with $\Lambda = 200\xi^{-1}$. The inset presents the extended Fröhlich model results up to $N_I = 100$ impurities.

transition occurred at significantly weaker coupling around $\alpha \approx 1$ for the lighter impurity at $m_b = 3.8m$. The regime shown in the figure can therefore still be considered as effectively a weak to intermediate coupling range what concerns the impurity localization properties.

In Chapter 3 we have shown that for a single impurity the extended Fröhlich effects start to become important once the polaronic contribution to the energy becomes negative, corresponding to the impurity getting localized. Indeed, in Figure 6.1 we can see that for $N_I = 1$ the difference in ground state energy between the Fröhlich and the extended Fröhlich model is rather small. This changes for multiple impurities where this difference between the two models becomes much more noticeable. While both models clearly predict a large multi-polaron binding energy, the extended Fröhlich model decreases the sharp drop of the energy per polaron to a much slower linear decrease. This is qualitatively consistent with the results obtained for a single impurity in Chapter 3. However, for multiple impurities this occurs at even weaker coupling when compared to the single polaron. This provides an important indication that the original Fröhlich model should not be used to analyze multiple impurities, even at weak coupling.

To confirm this, in Figure 6.2 we present results for the ground state energy per impurity at a fixed interaction strength as a function of the impurity number where the Aarhus experiment system parameters are used. At the coupling used in the figure $\alpha = 2.386$, the Fröhlich and extended Fröhlich models appear to be equivalent for a single impurity in Figure 6.1. However, it is now clearly evident that as the number of impurities increases, even at a fixed coupling the qualitative behavior of the two models drastically differs. While the Fröhlich model predicts a sharp increase in polaronic binding energy with growing number of impurities, the extended Fröhlich model severely restricts this behavior. Although the main plot of Figure 6.2 seems to indicate a quickly converged energy in the extended Fröhlich model, the inset shows that the energy still retains a weak dependence on N_I up to hundreds of impurities. The same plot is also presented in Figure 6.3 but now for the case of a light impurity $m_b = 3.8m$ that has been studied in Chapters 2 and 3, at $\alpha = 1$ with the remaining parameters as in [48]. Qualitatively identical behavior is obtained.

6.5 Impurity pockets in the extended Fröhlich model

The goal of the previous section was to compare the Fröhlich model and the extended Fröhlich model. We have thus far made two crucial observations. First, it is obvious that, even more so than for the case of a singly impurity, the extended Fröhlich model makes significant corrections to the Fröhlich model when multiple impurities are present. Second, in Figure 6.2 and Figure 6.3 we have seen that at some large number of impurities $N_I \approx 100$ the polaronic contribution to the ground state energy per impurity becomes practically indifferent to the addition of more impurities. In this section we will try to more closely understand this behavior.

It turns out that a simple but illuminating step towards understanding the behavior of the energy is to remember that the *full* Bose polaron energy is given by:

$$E = E_p + g_{ib} n_0 N_I \tag{6.49}$$

As discussed in Chapter 1, this value represents the true energy of the impurities with respect to the non-interacting state at $g_{ib} = 0$, which is also the quantity that is experimentally accessible. In fact, as can be seen from expression (6.21) it is far more natural to include this term in the energy when studying the extended Fröhlich model, as we have also done to perform the Lippmann-Schwinger regularization



FIGURE 6.4: Full polaron energy per impurity within the extended Fröhlich model for the system parameters of the Aarhus experiment [23], $m = m_b$ and $\Lambda \approx 190\xi^{-1}$ at zero temperature.

procedure. To avoid confusion, it is important to emphasize that the second term in (6.49) is completely independent of the polaronic state and all of our previous results for E_p remain completely valid and hence (6.49) is merely a trivial shift.

Nevertheless, it turns out that presenting the results of Figure 6.1 on a full energy plot provides quite some insight for a physical interpretation. This is done on Figure 6.4 where we have for comparison also added a larger number of impurities $N_I = 10$. We can now see that for a large number of impurities the full polaron energy per impurity is not only indifferent to further increasing the impurity number, but it is also very weakly dependent on the coupling strength. All of this seems to indicate that at sufficiently high impurity number, the impurities must be sharing a common depletion pocket in the condensate. The total energy in Figure 6.4 still remains positive, and this is therefore a metastable state in which the impurities are eventually preferably expelled out of the condensate. However, in realistic experiments harmonic trapping is used which may prevent expulsion of the impurities. This metastability is not something new, as the single polaron on the repulsive branch is also metastable in this sense. In this case, we know also that lower lying molecular states exist, and hence complete stability on the repulsive branch should not be expected to begin with.

A very similar prediction regarding impurity pockets has been made in a 2020

preprint by P. Naidon [120], where a mean-field like approach² has been used to analyze the properties of many impurities in the extended Fröhlich model. The author concludes that repulsive polarons might form polaron bubbles, situated in between full phase separation and a dilute mixture. However, more recently, a note has been added to this preprint that refers to a more general approach to this problem by the same author.

The more recent work cited in this note [121] approaches the problem from a completely different angle. The authors, now together with D. S Petrov who has authored the seminal work on BEC droplets [122], completely leave the polaronic point of view behind and approach the problem of bubbles relying on the similar ideas as in [122]. This work makes direct connection with the field of BEC mixtures which has recently gained a lot of renewed experimental [123-127] and theoretical [128–131] attention due to the observation of exotic droplet states in these systems. However, all of these studies approach the problem from a BEC-BEC mixture point of view, and the connection to a finite impurity polaronic limit is not always completely clear. For example, to the best of our knowledge none of the approaches made the connection to the Fröhlich model in the limit of weak coupling g_{ib} for $N_I = 1$, which is known to be valid at weak coupling for a single impurity. On the other hand, making the connection to the BEC mixture limit lies beyond the scope of the final chapter of the current thesis, as a completely new methodology would have to be used. For this reason we proceed within the polaronic point of view, but leave open the possibility that in the large N_I limit the quantum fluctuations arising from weak impurity-impurity interactions, which are completely neglected here, could become of importance, as seems to be the case in the mixture methods [128–131]. In general, the connection between the finite impurity limit and the mixtures limit is not completely clear and hence we believe the multi-polaron treatment to be an important first step towards establishing this link.

To confirm our suspicion that we are indeed dealing with an impurity cloud of a limited size, let us present the results for the impurity separation radius (6.47) in Figure 6.5. In the extended model we can see that between 5 impurities and 50 impurities, the average distance has barely changed which seems to support our claim that the impurities form a localized cloud. This can also been seen on the radial two-point density profile $g(\mathbf{r})$ on the right panel. It is interesting to note that Figure 6.5 provides further insight into the pathology of the Fröhlich model for multiple polarons. In the limit of $N_I \to \infty$ the impurities appear to collapse

²Different from Lee-Low-Pines theory



FIGURE 6.5: The average distance between each impurity compared between the Fröhlich and the extended Fröhlich model on the left panel (a) and the radial two-point density profile of the extended Fröhlich results on the right panel (b). The system parameters of the Aarhus experiment [23] are used with $m = m_b$ and $\Lambda \approx 190\xi^{-1}$ at zero temperature and coupling strength $(k_n a_{ib})^{-1} = 1.6.$

into a highly dense and tightly bound structure. Since the impurities themselves are non-interacting in our approach, the stabilization obtained in the extended model therefore arises purely from the condensate.

Finally, let us consider the question of how these many-polaron effects would look on an experimental scale for the repulsive branch in comparison with the data obtained in the Aarhus [23] experiment. This experimental data has more recently been adjusted to also account for the fact that on the repulsive branch the impurities move towards lower condensate densities [46], which we will refer to as the "modified Aarhus data". To the best of our knowledge, any potential binding effects between impurities have not been taken into account in the modified Aarhus analysis, but for completeness we will also present this data for comparison.

So far we were largely interested in the energy per polaron, which is the most convenient measure for comparing different impurity numbers on a single graph. However, if the many impurity state is tightly bound together and localized in



Mod. data Aarhus

 $(a_{ib}k_n)^{-1}$

1.5

 $\mathbf{2}$

2.5

FIGURE 6.6: Full polaron ground state energy per impurity within the extended Fröhlich model for the system parameters of the Aarhus experiment [23], $m = m_b$ and $\Lambda \approx 190\xi^{-1}$ at zero temperature. Data for the repulsive branch taken from Fig. 4 of [46].

1

Data Aarhus

0.5

-0.2

space as seen from the previous discussions, then the spectroscopic signal should be picking up on the total energy of the many-polaron state rather than the energy per impurity. On the other hand if the impurities are completely delocalized and uncorrelated one would rather expect the signal of relevance to be at the level of the single polaron E/N_I . An accurate analysis of how the radio signal interacts with the polaron state is beyond the scope of the current chapter, and requires access to the dynamics of the system. Therefore for our final comparison we will carefully proceed with the assumption that once the impurities start binding together, the relevant energy for comparison with experiment is the total many-polaron energy E, not divided by the impurity number. From the calculations in Figure 6.1 we can estimate that roughly around $\alpha \approx 1$ the binding energy of $N_I = 2$ impurities starts becoming discernible from the $N_I = 1$ state. Therefore we start our comparison to the experiment around $(k_n a_{ib})^{-1} = 2.5$ corresponding to $\alpha = 0.97$. For weaker interactions before this point, the single polaron QMC energy is in relatively good agreement with the modified data either way [46].

The results are presented on Figure 6.6 for a couple of different impurity numbers. As has been previously discussed in Chapter 3, we can immediately observe that the single polaron energy shows noticeable discrepancies from the



FIGURE 6.7: Color map of the polaron binding energy per particle $(E(N_I) - N_I E(1)) / [N_I \hbar^2 k_n^2 / (2m)]$ in the extended Fröhlich model in parameters of the Aarhus experiment [23], $m = m_b$ and $\Lambda \approx 190\xi^{-1}$ at zero temperature.

experimental data. Note that in the RG approach to the extended Fröhlich Hamiltonian [70], the same discrepancy is seen in this regime for a single polaron at zero temperature and hence this discrepancy is not inherent to our approach. We can see on the figure that for multiple impurities the energy signature is shifted upwards, and in particular around $N_I = 2$ similar energy scales as observed in the Aarhus experiment are to be expected. Our result indicates that if multipolaron $E = \sum_n w_n E_n$ contributions would be appropriately taken into account in a weighted average, the prediction for the spectroscopic energy following from a complete theoretical calculation would shift upwards. In Figure 6.7 we also present the polaron binding energy per particle to provide an estimate of the magnitude of the many polaron effects on the energy. As expected, the largest binding energy is observed at strong coupling and many impurities.

It is important to emphasize that there is currently no evidence that the measurements of the experiment contain bipolaron or higher multipolaron signals. For this reason we present Figure 6.6 mainly with the purpose of indicating how multipolaron signatures would look in the measurements, rather than a suggestion that many polaron effects are measured in the Aarhus experiment. In Figure 2 of the Aarhus experiment paper [23], the directly measured spectroscopic data is presented. In the regime that we are currently discussing, only the spectroscopic

signal at $(k_n a_{ib})^{-1} = 1.6$ was reported. From this signal it is clear that higher order many polaron peaks for $N_I > 2$ are not visible in the signal in any discernible way from the noise. However, the data points of the main peak at this coupling strength are quite broadened and noisy, and at least in principle could cover the energy scales of two peaks.

Nevertheless, there are many other effects that the discrepancy can be attributed to. Quantum Monte Carlo calculations for a single impurity, when accounting for higher order phonon-phonon interactions not present in the extended Fröhlich model [46] slightly shift the single polaron repulsive branch energy upwards, which partially but not completely eliminates the discrepancy. It has furthermore been shown in a mean field theory that finite temperature effects associated with condensate depletion can also increase the energy such that a better agreement with experiment is obtained [102], although we emphasize that beyond mean field effects are quite important at strong coupling.

6.6 Conclusion

In this final chapter we have combined different techniques from previous parts of this thesis to study the ground state properties of multiple impurities in a condensate. To describe the impurities we have proposed using the extended Fröhlich Hamiltonian that has been introduced and thoroughly discussed for a single polaron in Chapter 3. The tool of choice to tackle this problem has once again been the variational path integral approach. We have used results from Chapter 4 and Chapter 5 to argue that if the impurities are bosonic, then for the variational inequality at zero temperature distinguishable particles can be used in the variational model action. This allowed us to obtain the multiple impurity extension of the general memory kernel method, that was shown to be highly accurate in Chapter 2.

Previously, we have found that for a single impurity it is important to correct the Bogoliubov-Fröhlich Hamiltonian with its extended version once the coupling to the condensate becomes appreciable. Here, we find that this is even more the case in the presence of multiple impurities. While the Bogoliubov-Fröhlich Hamiltonian appears to predict extremely strongly bound and highly dense many impurity states with an ever increasing binding energy as the number of impurities grow, the extended Fröhlich model modifies this behavior such that a finite energy per particle is obtained in the $N_I \rightarrow \infty$ limit with a finite inter-impurity distance.

Finally we have also made a prediction as to how many polaron energy signatures on the repulsive branch would look in comparison to current experimental measurements. We predict a significant binding energy for the multipolaron state at strong coupling that definitely would fall in the measurable range of future experiments. In particular, we find that at intermediate to strong coupling, the bipolaron branch is quite close to the original experimental energy data points. This raises the question as to why such signals have not been observed in current experiments and provides further motivation, as already expressed by experimentalists, to investigate this interesting question more closely.

$_{\rm CHAPTER} 7$

Conclusions and outlook

Conclusions

For many decades now an intimate link existed between polaron physics and the path integral method, which provides a particularly simple description yielding remarkable accurate results at all polaronic regimes. The supremacy of the path integral method has been questioned with the advent of the novel Bose polaron problem. Bose polarons present a new set of theoretical challenges which can be roughly divided in three categories:

- (1) The Bose polaron appears to be a far more quantum mechanical object than its solid state counterpart, as the phonons become highly entangled even in the simplest weak coupling models [57, 64, 68, 69, 83]. To capture this system, older theoretic polaron descriptions have to be improved or fine-tuned.
- (2) As the coupling to the condensate becomes stronger, at the very least next-order scattering events between the impurity and the phonons have to be taken into account in the extended Fröhlich Hamiltonian [45, 49, 50, 70]. Similar contributions have only recently been encountered in other polaronic systems [91].
- (3) In the Bose polaron experiments [19, 23] the impurities are created at finite non-negligible number that can be controlled, providing a new ground for exploring many polaron effects.

Whereas quite some advances have already been made regarding the first point, the second and third points still form an area of active research with multiple open questions. Moreover, at the start of this thesis research, no clear direction existed

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as to how these challenges could be addressed within the path integral approach, which has proven to be a powerful tool in the past. The exploration of these topics has precisely been the goal of this thesis.

The first issue was explored in Chapter 2, where it was shown that the crucial step of improvement to capture the subtle phonon entanglement in the path integral approach is to provide the model action with more variational freedom through the use of general memory kernels. If perturbative corrections beyond the first-order inequality are accounted for on top of the variational solution, excellent agreement with diagrammatic Monte Carlo results is obtained.

The next challenge, namely including higher-order phonon scattering processes in the effective polaron action, was addressed in Chapter 3. We have shown that if the phonon scattering events are written out as a perturbative series at the level of the effective action, a pattern for exact resummation can be recognized. This problem has been tackled later on from a more general approach to these terms [91], confirming our result. Unfortunately, it is not clear how the resulting effective action can be computed exactly for variational applications, and at this point, to proceed at a semi-analytical level, we have proposed a number of approximations resulting in an approximate expression for the effective action. These approximations can be a posteriori justified by noticing that an analytical variational solution can be obtained at weak coupling, which exactly corresponds to the Lee-Low-Pines mean field ground state of the extended Fröhlich Hamiltonian. This indicates that our approach captures the same processes as the mean-field approach, but treats them beyond the mean-field level.

Finally, to tackle the last and most difficult issue, namely the presence of multiple impurities, we have first made a diversion and developed techniques to perform many-body path integrals for bosons in the presence of general memory kernels in Chapter 4 and Chapter 5. Aside from the application to specifically the Bose polaron problem, these systems provide a completely new class of variational model systems that could be used to study other bosonic many body systems in the canonical ensemble. These methods are then applied in Chapter 6 to extend the description of multiple impurities in the extended Fröhlich Hamiltonian on the repulsive polaron branch. We find that at zero temperature the bosonic effects can be ignored what concerns the variational ground state energy and the impurities can be treated as distinguishable in the variational model system. This significantly simplifies the approach and allows us to study various ground state properties of multiple impurities and make several predictions of where to look for many

polaron effects in future experiments.

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Outlook

We close off this very last chapter by making a couple of suggestions for future studies in this domain. An important quantity throughout this thesis has been the effective action of the extended Fröhlich Hamiltonian. This effective action was derived relying on a number of approximations that have made a semi-analytic treatment possible, hereby providing a first step to analyzing beyond-Fröhlich Hamiltonians in the path integral approach. Although the results are physically sound, improvements beyond the random phase approximation, or a rigorous analysis of the neglected terms would be of great interest in the future. This has broader relevance than just for the Bose polaron, since similar beyond Fröhlich Hamiltonians were recently derived for solid state polarons. Having shown that the Bogoliubov-Fröhlich Hamiltonian can be treated with great accuracy in the improved general memory kernel path integral approach, tackling the extended Fröhlich Hamiltonian with comparable rigor would be the next natural step.

For this reason we suggest a future effort to obtain a diagrammatic or diffusive Monte Carlo description of the extended Fröhlich model. Such results would be highly valuable, even for a single impurity. Numerous papers have come out in the last couple of years analyzing this Hamiltonian using a wide range of methods [45, 49, 50, 70, 81, 132], including the approach presented in this thesis. Having some exact numerical data for comparison would allow one to benchmark different approximations, and could in addition provide insights for similar problems in solid state physics [91]. This has already been proven to be the case for the Bogoliubov-Fröhlich model, where unexpected results came out of the diagMC study that indicated the necessity of more advanced theoretical tools. It would therefore be of great interest for future Monte Carlo studies to consider this direction on both the attractive and repulsive polaron branch.

This immediately brings us to our next point. In this thesis we have not considered the effects of higher order phonon-phonon interactions beyond the Bogoliubov approximation, which could be of importance at strong coupling. In one dimensional polarons [94] it has been shown that the extended Fröhlich model qualitatively accurately captures the polaron state, but at strong coupling a quantitatively significant reduction in energy on the repulsive branch is obtained when including phonon-phonon interactions. When comparing QMC calculations [46] on the repulsive branch with extended Fröhlich approaches such as [70] or the ones in this thesis, it appears that in contrast to the 1D case, in 3D these interactions increase the polaron energy. We believe it would be interesting to thoroughly study the effect of the phonon-phonon terms on the three dimensional polaron and find the regimes where they become important. This avenue could be explored by including phonon-phonon interactions within current approaches that work for the extended Fröhlich model.

Finally, as mentioned before, there is growing interest in understanding many polaron effects in future experiments [25, 100]. In this thesis we presented a beyond mean field treatment of the ground state properties of multiple impurities, and found that the binding energy of multiple polarons on the strongly repulsive branch should definitely fall within the range of measurable frequencies in the experiment. However, there is currently no reason to believe that these effects are present in the data of the original Aarhus experiment [23]. This is indicative of the fact that the many polaron metastable ground state is not reached and dynamical experimental studies like in [100] as a function of impurity concentration would be highly valuable to understand this question.

APPENDIX A

Simplifying the second order correction

In this appendix the second order cumulant correction (2.37) of Chapter 2 is computed. Written out in its full form, the effective action is given by:

$$\tilde{\mathcal{S}}_{\text{eff}} = -\frac{1}{8\pi} \frac{\alpha}{4\pi\mu^2} \int \mathbf{d}\mathbf{k} V_{\mathbf{k}}^2 \int_0^\beta d\tau \int_0^\beta d\sigma \mathcal{G}_{\mathbf{k}}(\tau - \sigma) e^{i\mathbf{k} \cdot [\mathbf{r}(\tau) - \mathbf{r}(\sigma)]}.$$
 (A.1)

The expectation value of the effective action with respect to the model system can be written in terms of

$$\mathcal{F}_{\mathbf{k}}(\tau - \sigma) = \left\langle e^{i\mathbf{k} \cdot [\mathbf{r}(\tau) - \mathbf{r}(\sigma)]} \right\rangle, \tag{A.2}$$

 \mathbf{as}

$$\left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle = -\frac{\alpha}{4\pi\mu^2} \frac{1}{2} \int_0^\Lambda dk \ k^2 V_{\mathbf{k}}^2 \int_0^\beta d\tau \int_0^\beta d\sigma \mathcal{G}_{\mathbf{k}}(\tau - \sigma) \mathcal{F}_{\mathbf{k}}(\tau - \sigma). \tag{A.3}$$

Both $\mathcal{G}_{\mathbf{k}}(\tau - \sigma)$ and $\mathcal{F}_{\mathbf{k}}(\tau - \sigma)$ only depend on the difference $|\tau - \sigma|$ and are in addition β -periodic. This allows to simplify the expectation value of the effective action to:

$$\frac{1}{\beta} \left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle = -\frac{\alpha}{4\pi\mu^2} \int_0^\Lambda dk \ k^2 V_{\mathbf{k}}^2 \int_0^{\beta/2} du \mathcal{G}_{\mathbf{k}}(u) \mathcal{F}_{\mathbf{k}}(u). \tag{A.4}$$

As already seen in Sec. 2.3, for a general model action $\mathcal{F}_{\mathbf{k}}(u)$ is given by:

$$\mathcal{F}_{\mathbf{k}}(u) = \exp\left(-\frac{2k^2}{\beta}\sum_{n=1}^{\infty}\frac{1-\cos(\nu_n u)}{x_n+\nu_n^2}\right).$$
 (A.5)

The terms in the cumulant expansion (2.37) can be derived using the λ -trick that has also been used in Sec. 2.3. It is not difficult to show that if a scaling parameter $x \to \lambda x$ is introduced in the memory kernel, the last two terms of (2.37) can be CHAPTER A - SIMPLIFYING THE SECOND ORDER CORRECTION

written as:

$$\begin{split} & \frac{1}{2\beta} \left(\left\langle \tilde{\mathcal{S}}_{0}^{2} \right\rangle - \left\langle \tilde{\mathcal{S}}_{0} \right\rangle^{2} \right) = -\frac{1}{2} \left. \frac{\partial^{2} F_{0}^{(\lambda)}}{\partial \lambda^{2}} \right|_{\lambda=1}, \\ & \frac{1}{\beta} \left(\left\langle \tilde{\mathcal{S}}_{\text{eff}} \tilde{\mathcal{S}}_{0} \right\rangle - \left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle \left\langle \tilde{\mathcal{S}}_{0} \right\rangle \right) = -\frac{1}{\beta} \left. \frac{\partial \left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle_{\lambda}}{\partial \lambda} \right|_{\lambda=1} \end{split}$$

The expression for $F_0^{(\lambda)}$ is given by (2.15) and hence:

$$\frac{1}{2\beta} \left(\left\langle \tilde{\mathcal{S}}_0^2 \right\rangle - \left\langle \tilde{\mathcal{S}}_0 \right\rangle^2 \right) = \frac{3}{2\beta} \sum_{n=1}^{\infty} \frac{x_n^2}{\left(\nu_n^2 + x_n\right)^2}.$$
 (A.6)

Similarly, $\langle \tilde{S}_{\text{eff}} \rangle$ is given by Expr. (A.3). To include the λ -dependence, x_n is substituted by λx_n in the memory function $\mathcal{F}_{\mathbf{k}}(u)$ after which the derivative can be taken. This yields:

$$\frac{1}{\beta} \left(\left\langle \tilde{\mathcal{S}}_{\text{eff}} \tilde{\mathcal{S}}_{0} \right\rangle - \left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle \left\langle \tilde{\mathcal{S}}_{0} \right\rangle \right) = \frac{4}{\beta} \sum_{n=1} \frac{x_{n}}{(\nu_{n}^{2} + x_{n})^{2}} \\
\times \frac{\alpha}{4\pi\mu^{2}} \int_{0}^{\Lambda} dk \ k^{4} V_{\mathbf{k}}^{2} \int_{0}^{\beta/2} \sin\left(\frac{\nu_{n}u}{2}\right)^{2} \mathcal{G}_{\mathbf{k}}(u) \mathcal{F}_{\mathbf{k}}(u) du. \tag{A.7}$$

We can now recognize in (A.7) the right-hand side of the iterative equation (2.24). This means that if we are considering a perturbative correction on top of the memory kernel that solves (2.24), we can write:

$$\frac{1}{\beta} \left(\left\langle \tilde{\mathcal{S}}_{\text{eff}} \tilde{\mathcal{S}}_0 \right\rangle - \left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle \left\langle \tilde{\mathcal{S}}_0 \right\rangle \right) = \frac{3}{\beta} \sum_{n=1} \frac{x_n^2}{(\nu_n^2 + x_n)^2} \tag{A.8}$$

which yields for the full second order correction around the optimized model action:

$$\frac{1}{2\beta} \left\langle (\Delta \mathcal{S} - \langle \Delta \mathcal{S} \rangle)^2 \right\rangle = \frac{1}{2\beta} \left(\left\langle \tilde{\mathcal{S}}_{\text{eff}}^2 \right\rangle - \left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle^2 \right) - \frac{3}{2\beta} \sum_{n=1}^{\infty} \frac{x_n^2}{\left(\nu_n^2 + x_n\right)^2}.$$
(A.9)

Next, consider the variance of the effective action in the first square bracket of (A.9). The first term of the variance can be written as:

$$\left\langle \tilde{\mathcal{S}}_{\text{eff}}^2 \right\rangle = \frac{\pi^2}{(2\pi)^6} \left(\frac{\alpha}{4\mu^2} \right)^2 \int \mathbf{d}\mathbf{k} \int \mathbf{d}\mathbf{s} V_{\mathbf{k}}^2 V_{\mathbf{s}}^2 \int_0^\beta d\tau_1 \int_0^\beta d\sigma_1 \int_0^\beta d\tau_2 \int_0^\beta d\sigma_2 \\ \times \mathcal{G}_{\mathbf{k}}(\tau_1 - \sigma_1) \mathcal{G}_{\mathbf{s}}(\tau_2 - \sigma_2) \left\langle e^{i\mathbf{k} \cdot [\mathbf{r}(\tau_1) - \mathbf{r}(\sigma_1)] + i\mathbf{s} \cdot [\mathbf{r}(\tau_2) - \mathbf{r}(\sigma_2)]} \right\rangle.$$
(A.10)

The generating function result (2.10) can now be used to find:

$$\left\langle e^{i\mathbf{k}\cdot[\mathbf{r}(\tau_1)-\mathbf{r}(\sigma_1)]+i\mathbf{s}\cdot[\mathbf{r}(\tau_2)-\mathbf{r}(\sigma_2)]} \right\rangle = \mathcal{F}_{\mathbf{k}}(\tau_1-\sigma_1)\mathcal{F}_{\mathbf{s}}(\tau_2-\sigma_2)$$
$$\times \exp\left(-\frac{\mathbf{k}\cdot\mathbf{s}}{4}\zeta\left(\tau_1-\sigma_1,\tau_2-\sigma_2,\frac{\tau_1+\sigma_1-\tau_2-\sigma_2}{2}\right)\right), \qquad (A.11)$$

where ζ is given by:

$$\zeta(u_1, u_2, s) = \frac{32}{\beta} \sum_{n=1}^{\infty} \frac{\sin(\frac{\nu_n u_1}{2}) \sin(\frac{\nu_n u_2}{2}) \cos(\nu_n s)}{\nu_n^2 + x_n}.$$
 (A.12)

The angle between **k** and **s** can be integrated out in (A.10) immediately. In addition we can see that the imaginary time integrals in (A.10) contain four variables, whereas the integrand only depends on $\tau_1 - \sigma_1$, $\tau_2 - \sigma_2$ and $(\frac{\tau_1 + \sigma_1 - \tau_2 - \sigma_2}{2})$. This allows to remove one integration variable and through the use of symmetry in the limit $\beta \to \infty$ significantly simplify the integral in similar spirit to what is done in [79]. Note however that even when divided by β , the integral (A.10) will still contain a divergence as $\beta \to \infty$ which is exactly canceled by subtracting its mean squared. Therefore in the limit of $\beta \to \infty$ we take both (A.3) and (A.10) together and obtain:

$$\frac{1}{2\beta} \left(\left\langle \tilde{\mathcal{S}}_{\text{eff}}^2 \right\rangle - \left\langle \tilde{\mathcal{S}}_{\text{eff}} \right\rangle^2 \right) = \left(\frac{\alpha}{4\pi\mu^2} \right)^2 \int_0^\Lambda dk k^2 \int_0^\Lambda ds s^2 V_{\mathbf{k}}^2 V_{\mathbf{s}}^2 \int_0^{\beta/2} du_1 \int_0^{\beta/2} du_2 \\ \times \mathcal{G}_{\mathbf{k}}(u_1) \mathcal{G}_{\mathbf{s}}(u_2) \mathcal{F}_{\mathbf{k}}(u_1) \mathcal{F}_{\mathbf{s}}(u_2) \int_0^{\beta/2} dz \left(\frac{\sinh\left[\frac{ks}{4}\zeta(u_1, u_2, z)\right]}{\frac{ks}{4}\zeta(u_1, u_2, z)} - 1 \right).$$
(A.13)

Contrary to the expression in [78, 79], the quantity in the inner integral is a $\sinh(x)/x$ function rather than an $\arcsin(x)/x$ function due to the fact that the momentum integrals cannot be performed analytically. It will prove to be useful to replace the hyperbolic sine function by its Taylor expansion:

$$\frac{\sinh(x)}{x} = \sum_{n=0}^{\infty} \frac{x^{2n}}{(2n+1)!}$$
(A.14)

which yields

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$$\times \mathcal{G}_{\mathbf{k}}(u_1)\mathcal{G}_{\mathbf{s}}(u_2)\mathcal{F}_{\mathbf{k}}(u_1)\mathcal{F}_{\mathbf{s}}(u_2) \int_0^{\beta/2} dz \sum_{n=1}^\infty \frac{1}{(2n+1)!} \left(\frac{ks}{4}\zeta(u_1,u_2,z)\right)^{2n}.$$
 (A.15)

Let us also define the individual terms of the sum, and emphasize their dependence on the memory kernel $x(\nu)$:

$$\sigma_{n}[x(\nu)] = \frac{1}{(2n+1)!} \left(\frac{\alpha}{4\pi\mu^{2}}\right)^{2} \int_{0}^{\Lambda} dkk^{2} \int_{0}^{\Lambda} dss^{2} V_{\mathbf{k}}^{2} V_{\mathbf{s}}^{2} \times \int_{0}^{\beta/2} du_{1} \int_{0}^{\beta/2} du_{2} \mathcal{G}_{\mathbf{k}}(u_{1}) \mathcal{G}_{\mathbf{s}}(u_{2}) \mathcal{F}_{\mathbf{k}}(u_{1}) \mathcal{F}_{\mathbf{s}}(u_{2}) \int_{0}^{\beta/2} dz \left(\frac{ks}{4} \zeta(u_{1}, u_{2}, z)\right)^{2n},$$
(A.16)

such that the entire second order cumulant is written as:

$$\frac{1}{2\beta} \left\langle \left(\Delta \mathcal{S} - \left\langle \Delta \mathcal{S} \right\rangle_0\right)^2 \right\rangle_0 = \sum_{n=1}^\infty \sigma_n[x(\nu)] - \frac{3}{2\beta} \sum_{n=1}^\infty \frac{x_n^2}{\left(\nu_n^2 + x_n\right)^2}.$$
 (A.17)

Note that the second term in (A.17) was obtained by assuming an expansion around the optimal memory kernel action and hence the same has to be done for the rest of the terms. Unfortunately, for a(n) (optimized) memory kernel $x(\nu)$ that has no trivial expression we cannot analytically perform the five-fold integral in (A.15) or (A.16), which is difficult even numerically. The exception to this is the n = 1 expansion term:

$$\sigma_{1}[x(\nu)] = \frac{1}{6(4)^{2}} \left(\frac{\alpha}{4\pi\mu^{2}}\right)^{2} \int_{0}^{\Lambda} dk k^{4} \int_{0}^{\Lambda} ds s^{4} V_{\mathbf{k}}^{2} V_{\mathbf{s}}^{2} \\ \times \int_{0}^{\beta/2} du_{1} \int_{0}^{\beta/2} du_{2} \mathcal{G}_{\mathbf{k}}(u_{1}) \mathcal{G}_{\mathbf{s}}(u_{2}) \mathcal{F}_{\mathbf{k}}(u_{1}) \mathcal{F}_{\mathbf{s}}(u_{2}) \int_{0}^{\beta/2} dz \zeta(u_{1}, u_{2}, z)^{2}.$$
(A.18)

By substituting ζ as given in (A.12) and using the orthogonality of the cosine, the z integral can be performed:

$$\int_{0}^{\beta/2} dz \zeta(u_1, u_2, z)^2 = \frac{32^2}{4\beta} \sum_{n=1}^{\infty} \frac{\sin(\frac{\nu_n u_1}{2})^2 \sin(\frac{\nu_n u_2}{2})^2}{(\nu_n^2 + x_n)^2}.$$
 (A.19)

The remaining four-fold integral completely decouples in each term of the sum in (A.19) and can be slightly simplified to:

 $\sigma_1[x(\nu)] =$

$$\frac{3}{2\beta} \sum_{n=1}^{\infty} \frac{1}{(\nu_n^2 + x_n)^2} \left[\frac{\alpha}{3\pi\mu^2} \int_0^{\Lambda} dk k^4 V_{\mathbf{k}}^2 \int_0^{\beta/2} du \mathcal{G}_{\mathbf{k}}(u) \mathcal{F}_{\mathbf{k}}(u) \sin\left(\frac{\nu_n u}{2}\right)^2 \right]^2 \quad (A.20)$$

The integral inside the square brackets is once again exactly the right-hand side of the iterative equation (2.24) which means that for the optimal memory kernel:

$$\sigma_1[x(\nu)] = \frac{3}{2\beta} \sum_{n=1}^{\infty} \frac{x_n^2}{(\nu_n^2 + x_n)^2}$$
(A.21)

cancels with the contribution from the other terms in (A.17). For an expansion around the optimal memory kernel the second order cumulant is written as:

$$\frac{1}{2\beta} \left\langle (\Delta S - \langle \Delta S \rangle)^2 \right\rangle = \sum_{n=2}^{\infty} \sigma_n[x(\nu)].$$
 (A.22)

APPENDIX **B**

Approximating the second order correction

In this appendix we will obtain a semi-analytic expression for the second order correction within the approximation discussed in the main text of Sec. 2.5 in Chapter 2:

$$\frac{1}{2\beta} \left\langle \left(\Delta \mathcal{S} - \left\langle \Delta \mathcal{S} \right\rangle\right)^2 \right\rangle^{(\text{approx.})} = \sum_{n=2}^{\infty} \sigma_n[0]. \tag{B.1}$$

The fact that the memory kernel vanishes, significantly simplifies the integral. First, expression (A.16) is rewritten using the symmetry around $\beta/2$ to fold the u_1, u_2 integration domain in half:

$$\sigma_n[x(\nu)] = \frac{2}{4^{2n}} \frac{1}{(2n+1)!} \left(\frac{\alpha}{4\pi\mu^2}\right)^2 \int_0^{\Lambda} dk k^{2+2n} \int_0^{\Lambda} ds s^{2+2n} V_{\mathbf{k}}^2 V_{\mathbf{s}}^2$$
$$\times \int_0^{\beta/2} du_1 \int_0^{u_1} du_2 \mathcal{G}_{\mathbf{k}}(u_1) \mathcal{G}_{\mathbf{s}}(u_2) \mathcal{F}_{\mathbf{k}}(u_1) \mathcal{F}_{\mathbf{s}}(u_2) \int_0^{\beta/2} dz \zeta(u_1, u_2, z)^{2n}.$$
(B.2)

Next, observe that for $x(\nu) = 0$, the memory functions $\mathcal{F}_{\mathbf{k}}(u)$ simplify and in the limit of zero temperature this expression can be written as:

$$\sigma_{n}[0] = \frac{2}{4^{2n}} \frac{1}{(2n+1)!} \left(\frac{\alpha}{4\pi\mu^{2}}\right)^{2} \int_{0}^{\Lambda} dk k^{2+2n} \int_{0}^{\Lambda} ds s^{2+2n} V_{\mathbf{k}}^{2} V_{\mathbf{s}}^{2}$$
$$\times \int_{0}^{\beta/2} du_{1} \int_{0}^{u_{1}} du_{2} e^{-a(k)u_{1}} e^{-a(s)u_{2}} \int_{0}^{\beta/2} dz \zeta(u_{1}, u_{2}, z)^{2n}, \tag{B.3}$$

where the short hand notation with ω_k from (2.6) is introduced:

$$a(\mathbf{k}) = \omega_k + \frac{k^2}{2m}.\tag{B.4}$$

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As has already been observed in the weak-coupling limit of [79], in the absence of a memory kernel the expression for ζ becomes quite simple (note that our ζ is defined differently but the same structure holds):

$$\zeta(u_1, u_2, z) = \begin{cases} 4u_2 & \text{for } z < \frac{u_1 - u_2}{2}, \\ 2u_1 + 2u_2 - 4z & \text{for } \frac{u_1 - u_2}{2} < z < \frac{u_1 + u_2}{2}, \\ 0 & \text{for } \frac{u_1 + u_2}{2} < z. \end{cases}$$

The integral over z can now be analytically performed:

$$\int_{0}^{\beta/2} dz \zeta(u_1, u_2, z)^{2n} = 4^{2n} u_2^{2n} \frac{u_1 - u_2}{2} + 4^{2n} \frac{u_2^{2n+1}}{2n+1}.$$
 (B.5)

This allows to write (B.3) as:

$$\sigma_{n}[0] = \frac{2}{(2n+1)!} \left(\frac{\alpha}{4\pi\mu^{2}}\right)^{2} \int_{0}^{\Lambda} dk k^{2+2n} \int_{0}^{\Lambda} ds s^{2+2n} V_{\mathbf{k}}^{2} V_{\mathbf{s}}^{2}$$
$$\times \int_{0}^{\beta/2} du_{1} \int_{0}^{u_{1}} du_{2} e^{-a(k)u_{1}} e^{-a(s)u_{2}} \left[u_{2}^{2n} \frac{u_{1}-u_{2}}{2} + \frac{u_{2}^{2n+1}}{2n+1}\right].$$
(B.6)

The integrals over u_1 and u_2 are given by

$$\int_{0}^{\infty} du_{1} \int_{0}^{u_{1}} du_{2} e^{-a(\mathbf{k})u_{1}} e^{-a(\mathbf{s})u_{2}} \left[u_{2}^{2n} \frac{u_{1} - u_{2}}{2} + \frac{u_{2}^{2n+1}}{2n+1} \right]$$
$$= \frac{(3a(k) + a(s)) n\Gamma(2n)}{a(k)^{2} (a(k) + a(s))^{2+2n}}.$$
(B.7)

Since n is an integer $n\Gamma(2n) = (2n)!/2$ and therefore:

$$\sigma_n[0] = \frac{1}{(2n+1)} \left(\frac{\alpha}{4\pi\mu^2}\right)^2 \int_0^\Lambda dk \int_0^\Lambda ds V_{\mathbf{k}}^2 V_{\mathbf{s}}^2 \frac{k^{2+2n} s^{2+2n} \left(3a(k) + a(s)\right)}{a(k)^2 \left(a(k) + a(s)\right)^{2+2n}}.$$
 (B.8)

Finally, we can define

$$Q = \sum_{n=2}^{\infty} \frac{1}{(2n+1)} \left(\frac{1}{4\pi\mu^2}\right)^2 \int_0^{\Lambda} dk \int_0^{\Lambda} ds V_{\mathbf{k}}^2 V_{\mathbf{s}}^2 \frac{k^{2+2n} s^{2+2n} \left(3a(k) + a(s)\right)}{a(k)^2 \left(a(k) + a(s)\right)^{2+2n}}, \quad (B.9)$$

such that the full approximate second order correction is given by:

$$E_2 = -\alpha^2 Q. \tag{B.10}$$

APPENDIX C

Deriving the Lagrangian of the extended Fröhlich model

In this appendix we derive the classical Lagrangian corresponding to the extended Fröhlich Hamiltonian (3.1) at the heart of Chapter 3. The first step is to introduce the following operators associated with the phonon field:

$$\hat{Q}_{\mathbf{k}} = \sqrt{\frac{\hbar}{2M\omega(\mathbf{k})}} \left(\hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{-\mathbf{k}}^{\dagger} \right), \qquad (C.1)$$

$$\hat{P}_{\mathbf{k}} = i \sqrt{\frac{\hbar M \omega(\mathbf{k})}{2}} \left(\hat{\alpha}_{\mathbf{k}}^{\dagger} - \hat{\alpha}_{-\mathbf{k}} \right).$$
(C.2)

The operators can be easily confirmed to obey the commutation relations $\left[\hat{Q}_{\mathbf{k}}, \hat{P}_{\mathbf{k}'}\right] = i\hbar \delta_{\mathbf{k},\mathbf{k}'}$ and hence can be interpreted as position and momentum variables associated with the phonon field. As also the case in [62], the operators are not completely hermitian $\hat{Q}_{\mathbf{k}}^{\dagger} = \hat{Q}_{-\mathbf{k}}$, $\hat{P}_{\mathbf{k}}^{\dagger} = \hat{P}_{-\mathbf{k}}$ which implies that their associated scalar variables can be complex. For the purpose of dimensionality, in expressions (C.1) and (C.2), a completely arbitrary phonon mass M has been introduced which will vanish in all physically relevant expressions and is not to be confused with the model action mass M in Feynman's model. On the other hand, the frequency in $\hbar \omega_{\mathbf{k}} = \epsilon(\mathbf{k})$ in (C.1) corresponds to the Bogoliubov energy dispersion and plays an important role in the problem.

In terms of the new operators $\hat{Q}_{\mathbf{k}}$ and $\hat{P}_{\mathbf{k}}$ the extended Fröhlich Hamiltonian can be written as:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \sum_{\mathbf{k}} \frac{M\omega_{\mathbf{k}}^2}{2} \hat{Q}_{\mathbf{k}}^{\dagger} \hat{Q}_{\mathbf{k}} + \sum_{\mathbf{k}} \frac{1}{2M} \hat{P}_{\mathbf{k}}^{\dagger} \hat{P}_{\mathbf{k}} + \frac{\sqrt{N_0} g_{ib}}{V} \sum_{\mathbf{k} \neq \mathbf{0}} \hat{\rho}_{\mathbf{k}} \sqrt{\frac{2M\omega_{\mathbf{k}}}{\hbar}} V_{\mathbf{k}} \hat{Q}_{\mathbf{k}}$$

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$$+\frac{g_{ib}}{V}\sum_{\mathbf{k},\mathbf{s}}\hat{\rho}_{\mathbf{k}-\mathbf{s}}V_{\mathbf{k}}V_{\mathbf{s}}\frac{M\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}}{2\hbar}\hat{Q}_{\mathbf{s}}^{\dagger}\hat{Q}_{\mathbf{k}} + \frac{g_{ib}}{V}\sum_{\mathbf{k},\mathbf{s}}\hat{\rho}_{\mathbf{k}-\mathbf{s}}V_{\mathbf{k}}^{-1}V_{\mathbf{s}}^{-1}\frac{1}{2M\hbar\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}}\hat{P}_{\mathbf{k}}^{\dagger}\hat{P}_{\mathbf{s}}.$$
(C.3)

Two types of diverging terms containing the commutator $\begin{bmatrix} \hat{Q}_{\mathbf{k}}, \hat{P}_{\mathbf{k}} \end{bmatrix}$ arise in the derivation of (C.3). The first one corresponds to the ground-state energy of the introduced harmonic oscillators $-\sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}}/2$. The other one arises from the cross terms in the extended interactions and is given by $-\frac{g_{ib}}{2V}\sum_{\mathbf{k}} W_{\mathbf{k},\mathbf{k}}^{(1)}$. This term contains a UV divergence that can not be regularized by taking the cutoff-dependence of g_{ib} into account. Neither of these terms contains the impurity coordinate and we will not include them in further discussion. The classical Hamiltonian corresponding to (C.3) is now obtained by replacing the operators with complex scalar variables that obey $Q_{\mathbf{k}}^* = Q_{-\mathbf{k}}$:

$$H = \frac{\mathbf{p}^2}{2m} + \sum_{\mathbf{k}} \frac{M\omega_{\mathbf{k}}^2}{2} Q_{-\mathbf{k}} Q_{\mathbf{k}} + \sum_{\mathbf{k}} \frac{1}{2M} P_{-\mathbf{k}} P_{\mathbf{k}} + \frac{\sqrt{N_0} g_{ib}}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \rho_{\mathbf{k}} \sqrt{\frac{2M\omega_{\mathbf{k}}}{\hbar}} V_{\mathbf{k}} Q_{\mathbf{k}} + \frac{g_{ib}}{V} \sum_{\mathbf{k},\mathbf{s}} \rho_{\mathbf{k}-\mathbf{s}} V_{\mathbf{k}} V_{\mathbf{s}} \frac{M\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}}{2\hbar} Q_{-\mathbf{s}} Q_{\mathbf{k}} + \frac{g_{ib}}{V} \sum_{\mathbf{k},\mathbf{s}} \rho_{\mathbf{k}-\mathbf{s}} V_{\mathbf{k}}^{-1} V_{\mathbf{s}}^{-1} \frac{1}{2M\hbar\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}} P_{-\mathbf{k}} P_{\mathbf{s}}.$$
(C.4)

The Legendre transformation:

$$L = \sum_{\mathbf{q}} \frac{\partial H}{\partial P_{\mathbf{q}}} P_{\mathbf{q}} + \frac{\partial H}{\partial \mathbf{p}} \cdot \mathbf{p} - H$$
(C.5)

results in the classical Lagrangian:

$$L = \frac{m\dot{\mathbf{r}}^2}{2} - \sum_{\mathbf{k}} \frac{M\omega_{\mathbf{k}}^2}{2} Q_{-\mathbf{k}} Q_{\mathbf{k}} + \sum_{\mathbf{k}} \frac{1}{2M} P_{-\mathbf{k}} P_{\mathbf{k}} - \frac{\sqrt{N_0} g_{ib}}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \rho_{\mathbf{k}} \sqrt{\frac{2M\omega_{\mathbf{k}}}{\hbar}} V_{\mathbf{k}} Q_{\mathbf{k}}$$
$$- \frac{g_{ib}}{V} \sum_{\mathbf{k},\mathbf{s}} \rho_{\mathbf{k}-\mathbf{s}} V_{\mathbf{k}} V_{\mathbf{s}} \frac{M\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}}{2\hbar} Q_{-\mathbf{s}} Q_{\mathbf{k}} + \frac{g_{ib}}{V} \sum_{\mathbf{k},\mathbf{s}} \rho_{\mathbf{k}-\mathbf{s}} V_{\mathbf{k}}^{-1} V_{\mathbf{s}}^{-1} \frac{1}{2M\hbar\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}} P_{-\mathbf{k}} P_{\mathbf{s}},$$
$$(C.6)$$

where the impurity coordinate \mathbf{r} has now been explicitly introduced. The Lagrangian (C.6) still has to be written as a function of the velocity of the phonon
variables by using:

$$\dot{Q}_{\mathbf{q}} = \frac{\partial H}{\partial P_{\mathbf{q}}} \implies P_{-\mathbf{k}} = M\dot{Q}_{\mathbf{k}} - \frac{g_{ib}}{V} \sum_{\mathbf{q}} \rho_{\mathbf{q}-\mathbf{k}} V_{\mathbf{q}}^{-1} V_{\mathbf{k}}^{-1} \frac{1}{\hbar\sqrt{\omega_{\mathbf{q}}\omega_{\mathbf{k}}}} P_{-\mathbf{q}}.$$
 (C.7)

To simplify the algebra we can multiply the RHS of (C.7) by $P_{\mathbf{k}}/(2M)$ and perform the summation over \mathbf{k} . The two momentum-dependent terms in the Lagrangian can then be compactly written as:

$$L = \frac{m\dot{\mathbf{r}}^2}{2} - \sum_{\mathbf{k}} \frac{M\omega_{\mathbf{k}}^2}{2} Q_{-\mathbf{k}} Q_{\mathbf{k}} + \sum_{\mathbf{k}} \frac{1}{2} \dot{Q}_{\mathbf{k}} P_{\mathbf{k}} - \frac{\sqrt{N_0} g_{ib}}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \rho_{\mathbf{k}} \sqrt{\frac{2M\omega_{\mathbf{k}}}{\hbar}} V_{\mathbf{k}} Q_{\mathbf{k}} - \frac{g_{ib}}{V} \sum_{\mathbf{k},\mathbf{s}} \rho_{\mathbf{k}-\mathbf{s}} V_{\mathbf{k}} V_{\mathbf{s}} \frac{M\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}}{2\hbar} Q_{-\mathbf{s}} Q_{\mathbf{k}}.$$
(C.8)

Next we shall look for an explicit expression for $P_{\mathbf{k}}$. Expression (C.7) can be equivalently written as:

$$P_{\mathbf{k}} = M\dot{Q}_{-\mathbf{k}} - \frac{g_{ib}}{V} \sum_{\mathbf{q}} \rho_{\mathbf{k}-\mathbf{q}} V_{\mathbf{q}}^{-1} V_{\mathbf{k}}^{-1} \frac{1}{\hbar\sqrt{\omega_{\mathbf{q}}\omega_{\mathbf{k}}}} P_{\mathbf{q}}.$$
 (C.9)

Note that for a single impurity $\rho_{\mathbf{k}-\mathbf{q}} = \rho_{\mathbf{k}}\rho_{-\mathbf{q}}$. By multiplying (C.9) with $\frac{V_{\mathbf{k}}^{-1}\rho_{-\mathbf{k}}}{\sqrt{\hbar\omega_{\mathbf{k}}}}$ and performing the summation over \mathbf{k} we find:

$$\sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{-1} \rho_{-\mathbf{k}}}{\sqrt{\hbar\omega_{\mathbf{k}}}} P_{\mathbf{k}} = \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{-1} \rho_{-\mathbf{k}}}{\sqrt{\hbar\omega_{\mathbf{k}}}} M \dot{Q}_{-\mathbf{k}} - \frac{g_{ib}}{V} \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{-2}}{\hbar\omega_{\mathbf{k}}} \sum_{\mathbf{q}} \frac{V_{\mathbf{q}}^{-1} \rho_{-\mathbf{q}}}{\sqrt{\hbar\omega_{\mathbf{q}}}} P_{\mathbf{q}}.$$
 (C.10)

Equation (C.10) can be algebraically solved to obtain:

$$\sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{-1} \rho_{-\mathbf{k}}}{\sqrt{\hbar\omega_{\mathbf{k}}}} P_{\mathbf{k}} = \eta \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{-1} \rho_{-\mathbf{k}}}{\sqrt{\hbar\omega_{\mathbf{k}}}} M \dot{Q}_{-\mathbf{k}}, \tag{C.11}$$

where $\eta = \left(1 + \frac{g_{ib}}{V} \sum_{\mathbf{k}} \frac{V_{\mathbf{k}}^{-2}}{\hbar \omega_{\mathbf{k}}}\right)^{-1}$. After substituting (C.11) into (C.9) the expression for $P_{\mathbf{k}}$ becomes:

$$P_{\mathbf{k}} = M\dot{Q}_{-\mathbf{k}} - \frac{g_{ib}}{V}M\eta \frac{V_{\mathbf{k}}^{-1}\rho_{\mathbf{k}}}{\sqrt{\hbar\omega_{\mathbf{q}}}} \sum_{\mathbf{q}} \frac{V_{\mathbf{q}}^{-1}\rho_{-\mathbf{q}}}{\sqrt{\hbar\omega_{\mathbf{q}}}}\dot{Q}_{-\mathbf{q}}.$$
 (C.12)

Finally we can substitute (C.12) in (C.8) to obtain the resulting Lagrangian of the

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extended Fröhlich model:

$$L = \frac{m\dot{\mathbf{r}}^2}{2} + \frac{M}{2} \sum_{\mathbf{k}} \dot{Q}_{\mathbf{k}} \dot{Q}_{-\mathbf{k}} - \sum_{\mathbf{k}} \frac{M\omega_{\mathbf{k}}^2}{2} Q_{-\mathbf{k}} Q_{\mathbf{k}} - \frac{\sqrt{N_0} g_{ib}}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \rho_{\mathbf{k}} \sqrt{\frac{2M\omega_{\mathbf{k}}}{\hbar}} V_{\mathbf{k}} Q_{\mathbf{k}}$$
$$- \frac{g_{ib}}{V} \frac{M}{2} \sum_{\mathbf{k},\mathbf{s}} \rho_{\mathbf{k}-\mathbf{s}} V_{\mathbf{k}} V_{\mathbf{s}} \frac{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}}{\hbar} Q_{-\mathbf{s}} Q_{\mathbf{k}} - \frac{g_{ib}}{V} \frac{M\eta}{2} \sum_{\mathbf{k},\mathbf{s}} \frac{V_{\mathbf{k}}^{-1} V_{\mathbf{s}}^{-1}}{\hbar \sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{s}}}} \rho_{\mathbf{k}-\mathbf{s}} \dot{Q}_{\mathbf{k}} \dot{Q}_{-\mathbf{s}}.$$
(C.13)

APPENDIX D

Derivation of the distinguishable particle propagator

In this appendix the factorization of the many-body propagator (4.6) discussed in Chapter 4 will be proven. For the single-particle limit of (4.1), the classical action is calculated in [113]. For completeness and due to slightly different notations, we briefly summarize the calculation below. Consider the single-particle action functional:

$$S^{(1)}[\mathbf{r}, x, \boldsymbol{\kappa}] = \int_0^\beta \frac{m\dot{\mathbf{r}}^2}{2} dt + \frac{m}{2} \int_0^\beta d\tau \int_0^\beta d\sigma x(\tau - \sigma) \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma) - m \int_0^\beta d\tau \mathbf{r}(\tau) \cdot \boldsymbol{\kappa}(\tau) \cdot \mathbf{r}(\tau) \cdot \mathbf{r}(\sigma) d\tau \mathbf{r}(\tau) \cdot \mathbf{r}$$

The classical path is found as the solution to the following integro-differential equation with boundary conditions $\mathbf{r}_T = \mathbf{r}(\beta)$ and $\mathbf{r}_0 = \mathbf{r}(0)$:

$$\ddot{\mathbf{r}}(\tau) - \int_0^\beta x(t-\sigma)\mathbf{r}(\sigma)d\sigma + \boldsymbol{\kappa}(\tau) = 0.$$
 (D.2)

In [113], the following Fourier decomposition is proposed:

$$\mathbf{r}_{\rm cl}(\tau) = \mathbf{r}_0 + (\mathbf{r}_T - \mathbf{r}_0)\frac{\tau}{\beta} - \frac{\mathbf{A}_0}{2}\tau(\tau - \beta) + \sum_{n \neq 0} \frac{\mathbf{A}_n}{\nu_n^2} \left(e^{i\nu_n\tau} - 1\right),\tag{D.3}$$

where after substitution into (D.2), the following solutions are found (assuming $x_0 \neq 0$, otherwise the appropriate limit should be taken):

$$\mathbf{A}_{0} = \frac{4}{\beta^{2} \Delta_{x}} \left(\sum_{n} \frac{\boldsymbol{\kappa}_{n}}{\nu_{n}^{2} + \beta x_{n}} - \frac{1}{2} (\mathbf{r}_{T} + \mathbf{r}_{0}) \right), \tag{D.4}$$

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$$\mathbf{A}_{n} = \frac{\beta x_{n}}{\nu_{n}^{2} + \beta x_{n}} \mathbf{A}_{0} + \frac{1}{\left(1 + \frac{\beta x_{n}}{\nu_{n}^{2}}\right)} \left(\boldsymbol{\kappa}_{n} + x_{n} \frac{\mathbf{r}_{T} - \mathbf{r}_{0}}{i\nu_{n}}\right).$$
(D.5)

The coefficients can be substituted into (D.3) to obtain an explicit expression for the classical solution $\mathbf{r}_{cl}(\tau)$ and its Fourier components \mathbf{r}_n . After integrating the kinetic energy by parts, and writing the remaining source term integral in Fourier space, the classical action can be written as:

$$S_{\rm cl}^{(1)}[x,\boldsymbol{\kappa}](\mathbf{r}_T,\mathbf{r}_0) = \frac{m}{2} \left(\dot{\mathbf{r}}_{\rm cl}(\beta) \mathbf{r}_T - \dot{\mathbf{r}}_{\rm cl}(0) \mathbf{r}_0 \right) - \frac{m\beta}{2} \sum_n \mathbf{r}_n \cdot \boldsymbol{\kappa}_{-n}.$$
 (D.6)

By taking the derivative of (D.3) and substituting its boundary points to find the first part, and performing the Fourier sum using $\mathbf{r}_n = \frac{\kappa_n - \mathbf{A}_n}{\beta x_n}$ to find the second part, the single-particle classical action becomes:

$$S_{\rm cl}^{(1)}[x,\boldsymbol{\kappa}](\mathbf{r}_T,\mathbf{r}_0) = \frac{m}{2\beta}A_x(\mathbf{r}_T-\mathbf{r}_0)^2 + \frac{m}{2\beta}\frac{1}{\Delta_x}(\mathbf{r}_T+\mathbf{r}_0)^2$$
$$-\frac{2m}{\beta}\frac{1}{\Delta_x}(\mathbf{r}_T+\mathbf{r}_0)\cdot\sum_n\frac{\boldsymbol{\kappa}_n}{\nu_n^2+\beta x_n} + \frac{2m}{\beta}(\mathbf{r}_T-\mathbf{r}_0)\cdot\left(\frac{\beta}{2}\sum_n\frac{i\nu_n\boldsymbol{\kappa}_n}{\nu_n^2+\beta x_n}\right)$$
$$+\frac{2m}{\beta}\frac{1}{\Delta_x}\left(\sum_n\frac{\boldsymbol{\kappa}_n}{\nu_n^2+\beta x_n}\right)^2 - \frac{2m}{\beta}\left(\frac{\beta^2}{4}\sum_n\frac{\boldsymbol{\kappa}_n\cdot\boldsymbol{\kappa}_{-n}}{\nu_n^2+\beta x_n}\right).$$
(D.7)

For the source terms, some care should be taken regarding point-wise convergence when performing calculations in Fourier space, as pointed out in [113]. For example, when considering a source function $\kappa(\tau) = f\delta(\tau - \sigma)$ for $\sigma = 0$ or $\sigma = \beta$, the correct result should be derived by considering $\sigma \in]0, \beta[$ and respectively taking the limit of $\sigma \to 0^+$ or $\sigma \to \beta^-$ rather than direct substitution due to discontinuities at the edge. Taking care of the appropriate limits, the known results for e.g. the harmonic oscillator or the kicked particle are readily obtained from (D.7).

To obtain the many-particle extension of this result for the action functional (4.1), a similar but lengthier calculation was performed starting from equations (4.4) and (4.5) by first finding $\mathbf{R}_{cl}(\tau)$ with the previous method and then using this result to solve the equation for $\mathbf{r}_{cl}^{(i)}(\tau)$. However, in line with [107], a somewhat shorter argument yielding the same result can be formulated by switching to the

variable $\mathbf{u}_i = \mathbf{r}_i - \mathbf{R}$ at the level of the classical equations:

$$\ddot{\mathbf{R}}(\tau) - \int_{0}^{\beta} y(\tau - \sigma) \mathbf{R}(\sigma) d\sigma + \mathbf{K}(\tau) = 0, \qquad (D.8)$$

$$\ddot{\mathbf{u}}_{i}(\tau) - \int_{0}^{\beta} x(t-\sigma)\mathbf{u}_{i}(\sigma)d\sigma + \boldsymbol{\kappa}_{i}(\tau) - \mathbf{K}(\tau) = 0, \qquad (D.9)$$

with boundary conditions $\mathbf{u}_{i,(T,0)} = \mathbf{r}_{i,(T,0)} - \mathbf{R}_{(T,0)}$. In addition, the solution is subject to the constraint $\sum_i \mathbf{u}_i(\tau) = \mathbf{0}$. The many-body classical action corresponding to (4.1), written in terms of the coordinates \mathbf{u}_i and \mathbf{R} yields:

$$S_{\rm cl}\left[x, y, \overline{\boldsymbol{\kappa}}\right]\left(\overline{\mathbf{r}}_T, \overline{\mathbf{r}}_0\right) = \sum_{i=1}^N S_{\rm cl}^{(1)}\left[x, \boldsymbol{\kappa}_i - \mathbf{K}\right]\left(\mathbf{u}_{i,T}, \mathbf{u}_{i,0}\right) + S_{\rm cl}^{(1)}\left[y, \sqrt{N}\mathbf{K}\right]\left(\sqrt{N}\mathbf{R}_T, \sqrt{N}\mathbf{R}_0\right).$$
(D.10)

Here, we have used the property $\sum_{i} \mathbf{u}_{i}(\tau) = \mathbf{0}$ to drop a number of terms, and add an additional source term in $\mathbf{K}(\tau)$ to obtain the difference of source terms $\boldsymbol{\kappa} - \mathbf{K}$ in the first term of (D.10). Through direct substitution of the boundary conditions $\mathbf{u}_{i,(T,0)} = \mathbf{r}_{i,(T,0)} - \mathbf{R}_{(T,0)}$ and source term $\boldsymbol{\kappa}_{i} - \mathbf{K}$ into (D.7), one can easily confirm that:

$$S_{\rm cl}\left[x, y, \overline{\boldsymbol{\kappa}}\right]\left(\overline{\mathbf{r}}_T, \overline{\mathbf{r}}_0\right) = \sum_{i=1}^N S_{\rm cl}^{(1)}\left[x, \boldsymbol{\kappa}_i\right]\left(\mathbf{r}_{i,T}, \mathbf{r}_{i,0}\right) + S_{\rm cl}^{(1)}\left[y, \sqrt{N}\mathbf{K}\right]\left(\sqrt{N}\mathbf{R}_T, \sqrt{N}\mathbf{R}_0\right) - S_{\rm cl}^{(1)}\left[x, \sqrt{N}\mathbf{K}\right]\left(\sqrt{N}\mathbf{R}_T, \sqrt{N}\mathbf{R}_0\right).$$
(D.11)

Next, we have to find the fluctuation factor of the propagator $K_N[x, y, \mathbf{0}](0, \beta|0, 0)$ as defined in Section 4.2. While the decomposition of the classical action (D.11) strongly suggests a similar factorization for the fluctuation factor, let us present a complete overview of the calculation. Following the approach in [113], we consider the many-particle fluctuation factor $K_N[\lambda x, \lambda y, \overline{\mathbf{0}}](0, \beta|0, 0)$ where the memory kernels are scaled by a variable λ , and define:

$$J(\lambda) = \log \left(K_N[\lambda x, \lambda y, \mathbf{0}](0, \beta | 0, 0) \right).$$
 (D.12)

The logarithm of the fluctuation factor J(1) can then be written as:

$$J(1) = J(0) + \int_0^1 d\lambda \frac{\partial J(\lambda)}{\partial \lambda} = J(0) + \int_0^1 d\lambda \frac{\frac{\partial}{\partial \lambda} K_N[\lambda x, \lambda y, \mathbf{0}](0, \beta | 0, 0)}{K_N[\lambda x, \lambda y, \mathbf{0}](0, \beta | 0, 0)}, \quad (D.13)$$

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where of course $J(0) = \frac{Nd}{2} \log\left(\frac{m}{2\pi\beta}\right)$ is the known free-particle result in d dimensions. In path-integral notation (4.2), one can write:

$$\frac{\partial}{\partial\lambda} K_{N}[\lambda x, \lambda y, \mathbf{0}](0, \beta | 0, 0)
= -\int_{0,0}^{0,\beta} \mathcal{D}\overline{\mathbf{r}} \left(\frac{m}{2} \sum_{i}^{N} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\sigma x(\tau - \sigma) \mathbf{r}_{\mathbf{i}}(\tau) \cdot \mathbf{r}_{\mathbf{i}}(\sigma)
+ \frac{m}{2N} \sum_{i,j} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\sigma \left[y(\tau - \sigma) - x(\tau - \sigma) \right] \mathbf{r}_{\mathbf{i}}(\tau) \cdot \mathbf{r}_{\mathbf{j}}(\sigma) \right) e^{-S^{(N)}[\overline{\mathbf{r}}, \lambda x, \lambda y, \mathbf{0}]}.$$
(D.14)

By making use of functional derivatives with respect to the source terms κ_i and taking them out of the path-integral, the propagator fraction in the λ -integral of (D.13) can be written as:

$$\frac{\frac{\partial}{\partial\lambda}K_{N}[\lambda x, \lambda y, \mathbf{0}](0, \beta | 0, 0)}{K_{N}[\lambda x, \lambda y, \mathbf{0}](0, \beta | 0, 0)} = -\left(\frac{1}{2m}\sum_{i}^{N}\int_{0}^{\beta}d\tau\int_{0}^{\beta}d\sigma x(\tau - \sigma)\frac{\partial}{\partial\boldsymbol{\kappa}^{(i)}(\tau)} \cdot \frac{\partial}{\partial\boldsymbol{\kappa}^{(i)}(\sigma)} + \frac{1}{2Nm}\int_{0}^{\beta}d\tau\int_{0}^{\beta}d\sigma \left[y(\tau - \sigma) - x(\tau - \sigma)\right]\sum_{i}\frac{\partial}{\partial\boldsymbol{\kappa}^{(i)}(\tau)} \cdot \sum_{j}\frac{\partial}{\partial\boldsymbol{\kappa}^{(j)}(\sigma)}\right) \times e^{-S_{\mathrm{cl}}[\lambda x, \lambda y, \overline{\kappa}](0, 0)}\Big|_{\boldsymbol{\kappa}^{\{i\}}=0}.$$
(D.15)

Since $S_{\rm cl} [\lambda x, \lambda y, \overline{\kappa}] (0, 0)$ is known, the functional derivatives can be straightforwardly performed to obtain:

$$\frac{\frac{\partial}{\partial\lambda}K_{N}[\lambda x, \lambda y, \mathbf{0}](0, \beta | 0, 0)}{K_{N}[\lambda x, \lambda y, \mathbf{0}](0, \beta | 0, 0)} = \frac{d}{2}(N-1)\left[\left(\sum_{n}\frac{1}{\nu_{n}^{2}+\lambda\beta x_{n}}\right)^{-1}\sum_{n}\frac{\beta x_{n}}{(\nu_{n}^{2}+\lambda\beta x_{n})^{2}} - \sum_{n}\frac{\beta x_{n}}{\nu_{n}^{2}+\lambda\beta x_{n}}\right] + \frac{d}{2}\left[\left(\sum_{n}\frac{1}{(\nu_{n}^{2}+\lambda\beta y_{n})^{2}}\right)^{-1}\sum_{n}\frac{\beta y_{n}}{(\nu_{n}^{2}+\lambda\beta y_{n})^{2}} - \sum_{n}\frac{\beta y_{n}}{\nu_{n}^{2}+\lambda\beta y_{n}}\right].$$
(D.16)

The λ -integral in (D.13) can now be analytically computed to finally obtain the many-body fluctuation factor:

$$K_N[x, y, \mathbf{0}](0, \beta | 0, 0) = K[x, \mathbf{0}](0, \beta | 0, 0)^{(N-1)} K[y, \mathbf{0}](0, \beta | 0, 0),$$
(D.17)

where the single-particle fluctuation factor in d dimensions is given by:

$$K[x, \mathbf{0}](0, \beta | 0, 0) = \left(\frac{m}{2\pi\beta}\right)^{\frac{d}{2}} \left(\frac{4}{\beta^3 x_0 \Delta_x}\right)^{\frac{d}{2}} \left(\frac{1}{\prod_{k=1}^{\infty} \left(1 + \frac{\beta x_k}{\nu_k^2}\right)}\right)^d.$$
(D.18)

This result together with (4.3) and (D.11) proves the factorization of the propagator in (4.6).

APPENDIX E

Explicit evaluation of closed loop Gaussian integrals

In this appendix we compute the Gaussian integral (4.18) in Chapter 4. Let us start by defining a shorthand notation for the single-particle propagator (4.9) with $\kappa_i = 0$:

$$K[x, \mathbf{0}](\mathbf{r}_T, \beta | \mathbf{r}_0, 0) = \mathcal{A}^d \exp\left(-a\left(\mathbf{r}_T - \mathbf{r}_0\right)^2 - b\left(\mathbf{r}_T + \mathbf{r}_0\right)^2\right), \qquad (E.1)$$

where $a = \frac{m}{2\beta}A_x$, $b = \frac{m}{2\beta}\frac{1}{\Delta_x}$, and:

$$\mathcal{A} = \left(\frac{m}{2\pi\beta}\right)^{1/2} \left(\frac{4}{\beta^3 x_0 \Delta_x}\right)^{1/2} \frac{1}{\prod_{k=1} \left(1 + \frac{\beta x_k}{\nu_k^2}\right)}.$$
(E.2)

It follows from expression (4.18) and (E.1) that the cyclic integral $h_{\ell}(\mathbf{k})$ factorizes as a product of each dimensional component $h_{\ell}(\mathbf{k}) = h_{\ell}(k_x)h_{\ell}(k_y)h_{\ell}(k_z)$, where each factor is of the form:

$$h_{\ell}(k_{z}) = \mathcal{A}^{\ell} \int_{-\infty}^{\infty} dz_{1} \dots \int_{-\infty}^{\infty} dz_{\ell} K[x,0](z_{1},\beta|z_{\ell},0) \dots K[x,0](z_{3},\beta|z_{2},0) \times K[x,0](z_{2},\beta|z_{1}0) e^{-i\frac{1}{N}k_{z}\sum_{j=1}^{\ell} z_{j}}.$$
 (E.3)

Here, the notation for $K[x, 0](z_1, \beta | z_\ell, 0)$ as a function of scalar points z_T and z_0 rather than vector variables refers to the propagator (E.1) in one dimension d = 1. After substitution of the propagators, expression (E.3) can also be calculated using the well-known Gaussian integral formula:

$$h_{\ell}(k_z) = \mathcal{A}^{\ell} \int_{-\infty}^{\infty} dz_1 \dots \int_{-\infty}^{\infty} dz_{\ell} \exp\left(-\mathbf{z}^T \mathcal{C} \mathbf{z} - \mathbf{B}^T \mathbf{z}\right)$$
$$= \mathcal{A}^{\ell} \sqrt{\frac{\pi^{\ell}}{\det(\mathcal{C})}} \exp\left(\frac{1}{4} \mathbf{B}^T \mathcal{C}^{-1} \mathbf{B}\right), \qquad (E.4)$$

where we invoke a vector notation for $\mathbf{z}^T = (z_1, ..., z_\ell)$, $\mathbf{B}^T = \frac{ik_z}{N}(1, ..., 1)$ and define the ℓ -dimensional matrix as:

$$C = \begin{pmatrix} 2(a+b) & (b-a) & 0 & \dots & (b-a) \\ (b-a) & 2(a+b) & (b-a) & \dots & \dots \\ 0 & (b-a) & 2(a+b) & \dots & 0 \\ \dots & \dots & \dots & \dots & (b-a) \\ (b-a) & \dots & 0 & (b-a) & 2(a+b) \end{pmatrix}.$$
 (E.5)

The matrix C is a circulant matrix, characterized by the property that any row or column is obtained by shifting the previous one by a single space (using periodic boundary conditions at the edges). Every circulant matrix has the same set of $j = \{0, 1, ..., \ell - 1\}$ eigenvectors [133]:

$$\mathbf{y}_j^T = \frac{1}{\sqrt{\ell}} \left(\rho_j^0, \rho_j^1, ..., \rho_j^{\ell-1} \right), \quad \text{where } \rho_j = e^{\frac{2\pi i}{\ell} j}, \tag{E.6}$$

with corresponding eigenvalues for this particular matrix [133]:

$$\lambda_j = 2(a+b) + 2(b-a)\cos\left(\frac{2\pi j}{\ell}\right).$$
(E.7)

The goal now is to calculate both the determinant of C and the quadratic form $\mathbf{B}^T C^{-1} \mathbf{B}$ of its inverse to obtain an explicit expression of (E.4). An expression for the determinant is readily written down as the product over all eigenvalues:

$$\det(\mathcal{C}) = \prod_{j=0}^{\ell-1} \left(2(a+b) + 2(b-a)\cos\left(\frac{2\pi j}{\ell}\right) \right)$$
$$= [2(a-b)]^{\ell} \prod_{j=0}^{\ell-1} \left(\frac{a+b}{a-b} - \cos\left(\frac{2\pi j}{\ell}\right) \right).$$
(E.8)

Consider the strictly positive real numbers a and b and assume $a \neq b$. We can now

define $\tilde{z} = \operatorname{arccosh}\left(\frac{a+b}{a-b}\right)$. For $\frac{a+b}{a-b} > 1$, \tilde{z} is real and uniquely defined. However, any $\frac{a+b}{a-b} < 1$ lies exactly on the branch cut of the arccosh-function, and \tilde{z} is complex and uniquely defined only up to the choice of whether the branch cut is approached from above or below the real axis. Either of the two choices work, and as we will show both yield the same result. Having converted $\frac{a+b}{a-b}$ in this form, the cosines in (E.8) can now be added:

$$\det(\mathcal{C}) = [2(a-b)]^{\ell} \prod_{j=0}^{\ell-1} \left(\cos(i\tilde{z}) - \cos\left(\frac{2\pi j}{\ell}\right) \right)$$
$$= [4(a-b)]^{\ell} \prod_{j=0}^{\ell-1} \sin\left(\frac{\pi j}{\ell} + \frac{i\tilde{z}}{2}\right) \prod_{j=0}^{\ell-1} \sin\left(\frac{\pi j}{\ell} - \frac{i\tilde{z}}{2}\right).$$
(E.9)

We encountered a very concise proof of the resulting sine product series in [134]. First note that the following polynomial in c can be decomposed in terms of its roots:

$$c^{\ell} - 1 = \prod_{j=0}^{\ell-1} \left(c - e^{\frac{2\pi i}{\ell}j} \right).$$
 (E.10)

Setting $c = e^{2iz}$, this can be applied to factorize the sine function as follows:

$$\sin(\ell z) = \frac{e^{-i\ell z}}{2i} \left(e^{2i\ell z} - 1 \right) = \frac{e^{-i\ell z}}{2i} \prod_{j=0}^{\ell-1} \left(e^{2iz} - e^{\frac{2\pi i}{\ell}j} \right).$$
(E.11)

After some algebraic manipulations on (E.11) one readily obtains for any complex z:

$$\prod_{j=0}^{\ell-1} \sin\left(\frac{\pi j}{\ell} + z\right) = \frac{1}{2^{\ell-1}} \sin(\ell z),$$
(E.12)

which is the known result found in tables of product series [135]. Using this result in (E.9) yields:

$$\det(\mathcal{C}) = 4 \left[(a-b) \right]^{\ell} \sinh\left(\frac{\ell}{2}\tilde{z}\right)^2.$$
 (E.13)

Let us now go back to the ambiguity of defining \tilde{z} along the branch cut. If $-1 < \frac{a+b}{a-b} < 1$, then \tilde{z} is purely imaginary and only changes sign across the branch

CHAPTER E - EXPLICIT EVALUATION OF CLOSED LOOP GAUSSIAN INTEGRALS

cut, which clearly doesn't affect (E.13). If $\frac{a+b}{a-b} < -1$, then the real part of \tilde{z} remains constant along the branch cut and the imaginary part jumps from π to $-\pi$, which does not change (E.13) for an integer ℓ . Therefore any choice gives the same result, and we can unambiguously write:

$$\det(\mathcal{C}) = 4 \left[(a-b) \right]^{\ell} \sinh\left(\frac{\ell}{2}\operatorname{arccosh}\left(\frac{a+b}{a-b}\right)\right)^2.$$
(E.14)

We want to emphasize that when a-b < 0 each of the two factors in (E.14) become negative for odd cycles ℓ , but the determinant always remains strictly positive and hence the square root in (E.4) is well defined and real.

Next we have to find the quadratic form of the inverse matrix $\mathbf{B}^T \mathcal{C}^{-1} \mathbf{B}$. For this, we note that the matrix \mathcal{C} is diagonalized as $D = Q^* \mathcal{C} Q$ [133], where Qis the matrix with the normalized eigenvectors (E.6), and D is the matrix with eigenvalues (E.7) on the diagonal. It readily follows that:

$$\mathbf{B}^{T} \mathcal{C}^{-1} \mathbf{B} = \mathbf{B}^{T} Q D^{-1} Q^{*} \mathbf{B} = -\frac{k_{z}^{2} \ell}{N^{2}} \frac{1}{4b}.$$
 (E.15)

The determinant (E.13) and quadratic form of the inverse (E.15) now yield:

$$h_{\ell}(k_z) = \mathcal{A}^{\ell} \left(\frac{\pi^{\ell}}{4 \left[(a-b) \right]^{\ell} \sinh\left(\frac{\ell}{2} \operatorname{arccosh}\left(\frac{a+b}{a-b}\right) \right)^2} \right)^{1/2} \exp\left(-\frac{k_z^2 \ell}{N^2} \frac{1}{16b}\right). \quad (E.16)$$

After substitution of a, b, A, and taking the dimensionality into account, we exactly obtain expression (4.19) in Section 4.3.

Appendix \mathbf{F}

Recurrence relation

To prove the recurrence relation in (4.23) of Chapter 4, consider the generating function:

$$G(u) = \sum_{n=0}^{\infty} \mathbb{Z}(n)u^n, \qquad (F.1)$$

with $\mathbb{Z}(n)$ as defined in (4.22). Remember that the summation in (4.22) restricts the coefficients to $\sum_{\ell=1}^{N} \ell M_{\ell} = N$, and hence the generating function can also be written as:

$$G(u) = \sum_{n=0}^{\infty} \sum_{M_1, M_2, \dots, M_n}^{*} \prod_{\ell=1}^{n} \frac{u^{\ell M_{\ell}}}{\ell^{M_{\ell}}(M_{\ell})!} \frac{1}{\left[2\sinh\left(\frac{\ell\beta\tilde{\Omega}}{2}\right)\right]^{M_{\ell}d}},$$
 (F.2)

where for short-hand notation we define $\beta \tilde{\Omega} = \operatorname{arccosh} \left[\frac{\Delta_{x_n}(0)A(x_n)+1}{\Delta_{x_n}(0)A(x_n)-1} \right]$. For any single term in n, and corresponding cycle decomposition $\{M_1, M_2, ..., M_n\}$, the product in (F.2) can be extended to infinity through multiplication by the trivial factors in $M_{n+1} = 0$, $M_{n+2} = 0$, ..., which corresponds to merely multiplying by ones. Hence for every finite set of numbers $V = \{M_1, M_2, ..., M_n\}$ appearing in (F.2), we can associate an infinite set $\tilde{V} = \{M_1, M_2, ..., M_\infty\} = \{V, 0, 0, 0, ...\}$. Now one can easily observe that the terms of (F.2) have a one-to-one mapping with all possible sets \tilde{V} . The following expression also has the same one-to-one mapping with all possible sets \tilde{V} and hence, assuming convergence, has to be the same:

$$G(u) = \prod_{\ell=1}^{\infty} \left(\sum_{M_{\ell}=0}^{\infty} \frac{u^{\ell M_{\ell}}}{\ell^{M_{\ell}}(M_{\ell})!} \frac{1}{\left[2\sinh\left(\frac{\ell\beta\tilde{\Omega}}{2}\right) \right]^{M_{\ell}d}} \right) = \exp\left(\sum_{\ell=1}^{\infty} \frac{u^{\ell}}{\ell \left[2\sinh\left(\frac{\ell\beta\tilde{\Omega}}{2}\right) \right]^{d}} \right).$$
(F.3)

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From (F.1) follows that:

$$\mathbb{Z}(N) = \left. \frac{1}{N!} \frac{d^{N-1}u}{du^{N-1}} \frac{d}{du} G(u) \right|_{u=0}.$$
 (F.4)

Applying this formula on the exponential form of (F.3), after some algebraic steps, readily yields the recurrence relation:

$$\mathbb{Z}(N) = \frac{1}{N} \sum_{k=0}^{N-1} \mathbb{Z}(k) \frac{1}{\left(2\sinh\left(\frac{(N-k)\beta\tilde{\Omega}}{2}\right)\right)^d}.$$
 (F.5)

$_{\rm appendix} \, G$

Calculation of the open cycle

In this appendix an expression for $O_{\ell}(\mathbf{k})$ given in (5.12) of Chapter 5 is computed. Since $O_{\ell}(\mathbf{k})$ factorizes in terms of its dimensional components it is sufficient to do the derivation in d = 1:

$$O_{\ell}(k) = \int dz_{2} \dots \int dz_{\ell} \ K[x](z',\beta|z_{\ell},0) \dots K[x](z_{3},\beta|z_{2},0) \times K[x](z_{2},\beta|z,0)e^{-\frac{i\mathbf{k}}{N} \cdot \sum_{j=2}^{\ell} z_{j}}.$$
 (G.1)

After substituting the expressions for the propagators (4.6) and performing the Gaussian integral we can write:

$$O_{\ell}(k) = \mathcal{A}^{\ell} \exp\left[-(a+b)(z'^{2}+z^{2})\right] \sqrt{\frac{\pi^{\ell-1}}{\det(\mathcal{T})}} \exp\left(\frac{1}{4}\left(c\mathbf{u}^{T}+\boldsymbol{\alpha}^{T}\right)\mathcal{T}^{-1}\left(c\mathbf{u}+\boldsymbol{\alpha}\right)\right),$$
(G.2)

where precisely as in Appendix E we use the shorthand notations $a = \frac{m}{2\beta}A_x$, $b = \frac{m}{2\beta}\frac{1}{\Delta_x}$. In addition we define the following vectors in (G.2): $\boldsymbol{\alpha}^T = (2(a - b)z, 0, ..., 0, 2(a - b)z')$, $\mathbf{z}^T = (z_2, z_3, ..., z_\ell)$, and $\mathbf{u}^T = (1, 1, ..., 1)$ with c = -ik/N. The main difference with the open cycles computed in Appendix E, corresponding to the calculations performed in Chapter 4, is that now the central object is the $(\ell - 1) \times (\ell - 1)$ dimensional tridiagonal Toeplitz matrix:

$$\mathcal{T} = \begin{pmatrix} 2(a+b) & (b-a) & 0 & \dots & 0\\ (b-a) & 2(a+b) & (b-a) & \dots & \dots\\ 0 & (b-a) & 2(a+b) & \dots & 0\\ \dots & \dots & \dots & \dots & (b-a)\\ 0 & \dots & 0 & (b-a) & 2(a+b) \end{pmatrix},$$
(G.3)

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which clearly loses the cyclic symmetry of the circulant matrices that appear in calculations of closed cycles.

The $j = \{1, ..., \ell - 1\}$ eigenvalues of the matrix \mathcal{T} are similar to those of the corresponding circulant matrix, but have a longer period in the cosine [136]:

$$\lambda_j = 2(a+b) + 2(b-a)\cos\left(\frac{j\pi}{\ell}\right). \tag{G.4}$$

The determinant of this matrix is then given by [137]:

$$\det(\mathcal{T}) = (a-b)^{\ell-1} U_{\ell-1}\left(\frac{a+b}{a-b}\right),\tag{G.5}$$

where $U_{\ell-1}\left(\frac{a+b}{a-b}\right)$ is the Chebyshev polynomial of the second kind. Here, we define $\zeta = \frac{a+b}{a-b}$ and restrict ourselves to strictly positive a and b with $a \neq b$. If a-b > 0 then $\zeta > 1$ and $U_{\ell-1}(\zeta)$ is strictly positive. If a-b < 0 then $\zeta < -1$ and $U_{\ell-1}(\zeta)$ can become negative for odd $\ell - 1$, which gets compensated by the additional negative sign from $(a-b)^{\ell-1}$. Therefore $\det(\mathcal{T})$ is always positive and well-defined.

For $|\zeta| > 1$ Chebyshev polynomials of the second kind can also be written as (with any choice of approaching the branch cut of the arccosh function):

$$U_{\ell-1}(\zeta) = \frac{\sinh(\ell \operatorname{arccosh}(\zeta))}{\sinh(\operatorname{arccosh}(\zeta))}.$$
 (G.6)

This yields the factor in front of (G.2), which leaves to find the quadratic form of the inverse in the exponent. The inverse elements of matrix \mathcal{T} are given by [137, 138] (where we have taken out an additional minus sign out of the Chebyshev polynomials):

$$T_{ij}^{-1} = \sigma_{ij} = \frac{1}{a-b} \frac{U_{i-1}(\zeta) U_{\ell-1-j}(\zeta)}{U_{\ell-1}(\zeta)} \quad \text{if} \quad i \le j,$$

$$T_{ij}^{-1} = \frac{1}{a-b} \frac{U_{j-1}(\zeta) U_{\ell-1-i}(\zeta)}{U_{\ell-1}(\zeta)} \quad \text{if} \quad i > j.$$

Since we have assumed a > 0 and b > 0 we can use the results of [138] to write:

$$\left(\mathcal{T}^{-1}\mathbf{u}\right)_{i} = s_{i} = \frac{1 + (b-a)(\sigma_{1,i} + \sigma_{1,\ell-i})}{4b} \quad \text{and} \quad \mathbf{u}^{T}\mathcal{T}^{-1}\mathbf{u} = \frac{(\ell-1) + 2(b-a)s_{1}}{4b}$$
(G.7)

This can now be used to compute all the necessary terms in the quadratic form in

the exponent of (G.2):

$$\mathbf{u}^{T} \mathcal{T}^{-1} \mathbf{u} = \frac{1}{4b} \left[\ell - \sqrt{\frac{a}{b}} \tanh\left(\frac{\ell}{2} \operatorname{arccosh}(\zeta)\right) \right], \tag{G.8}$$

$$\boldsymbol{\alpha}^{T} \mathcal{T}^{-1} \mathbf{u} = \left[\sqrt{\frac{a}{b}} \tanh\left(\frac{\ell}{2} \operatorname{arccosh}(\zeta)\right) - 1 \right] (z + z'), \tag{G.9}$$

$$\boldsymbol{\alpha}^{T} \mathcal{T}^{-1} \boldsymbol{\alpha} = \left(4(a+b) - 8\sqrt{ab} \tanh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)\right) (z^{2} + z'^{2}) - \frac{4(a-b)}{U_{\ell-1}(\zeta)} (z-z')^{2},$$
(G.10)

where we have used the easily proven identity:

$$\frac{U_{\ell-2}(\zeta)}{U_{\ell-1}(\zeta)} + \frac{1}{U_{\ell-1}(\zeta)} = \frac{a+b}{a-b} - \frac{2\sqrt{ab}}{a-b} \tanh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right).$$
(G.11)

Substituting both (G.5) and (G.8-G.10) into expression (G.2) finally yields:

$$O_{\ell}(k) = \mathcal{A}^{\ell} \sqrt{\frac{\pi^{\ell-1}}{(a-b)^{\ell-1} U_{\ell-1}(\zeta)}} \exp\left(-\frac{k^2}{16N^2 b} \left[\ell - \sqrt{\frac{a}{b}} \tanh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)\right] - \frac{ik}{2N} \left[\sqrt{\frac{a}{b}} \tanh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right) - 1\right] (z+z') - 2\sqrt{ab} \tanh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right) (z^2 + z'^2) - \frac{(a-b)}{U_{\ell-1}(\zeta)} (z-z')^2\right).$$
(G.12)

After substitution of a, b and A, and after generalization to d = 3 this yields exactly expression (5.13).

APPENDIX H

Calculation of the closed correlation cycles

In this appendix we will compute the two-point correlation cycle (5.28) of Chapter 5, which should also yield the one-point cycle (5.27) for $\kappa_2 = 0$. Quite similarly to Appendix G the computation is done in d = 1:

$$\chi_{\ell}(k,j) = \int dz_1 \dots \int dz_{\ell} \ e^{\tilde{a}_1(z_2+z_1)+\tilde{b}_1(z_2-z_1)} K[x](z_1,\beta|z_{\ell},0)\dots K[x](z_2,\beta|z_10)$$
$$e^{-\frac{ik}{N} \cdot \sum_{j=1}^{\ell} z_j} e^{\tilde{a}_2(z_{j+2}+z_{j+1})+\tilde{b}_2(z_{j+2}-z_{j+1})}, \tag{H.1}$$

and will be generalized at the end. Note that for $j = \ell - 1$ some care should be taken as z_{j+2} loops back to z_1 . In the derivation below we will implicitly assume $1 < j < \ell - 1$, but each step can be readily checked to hold for the boundary cases as well and the obtained result holds for any $1 \le j \le \ell - 1$. We can use the same notation for c, \mathbf{u} and \mathcal{A} as in Appendix G (but in ℓ dimensions) and define the vector:

$$\boldsymbol{w}_{j}^{T} = \left(\tilde{a}_{1} - \tilde{b}_{1}, \tilde{a}_{1} + \tilde{b}_{1}, 0, \dots, \tilde{a}_{2} - \tilde{b}_{2}, \tilde{a}_{2} + \tilde{b}_{2}, 0, \dots\right),$$
(H.2)

which has zeroes everywhere except for the positions: 1, 2, j + 1, j + 2. After substitution of the propagators, the Gaussian integral in (H.1) is readily performed:

$$\chi_{\ell}(k,j) = \mathcal{A}^{\ell} \sqrt{\frac{\pi^{\ell}}{\det(\mathcal{C})}} \exp\left(\frac{1}{4} \left(c\mathbf{u}^{T} + \boldsymbol{w}_{j}^{T}\right) \mathcal{C}^{-1} \left(c\mathbf{u} + \boldsymbol{w}_{j}\right)\right).$$
(H.3)

The cycle considered here is closed and hence just like in Chapter 4 and Appendix E the central object appearing is the $\ell \times \ell$ dimensional three-circulant

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matrix C that is defined by a periodic shifting of the first row:

$$\mathcal{C} = \operatorname{circ} \left(2(a+b), (b-a), 0, \dots, (b-a)\right) \\
= \begin{pmatrix} 2(a+b) & (b-a) & 0 & \dots & (b-a) \\ (b-a) & 2(a+b) & (b-a) & \dots & \dots \\ 0 & (b-a) & 2(a+b) & \dots & 0 \\ \dots & \dots & \dots & \dots & (b-a) \\ (b-a) & \dots & 0 & (b-a) & 2(a+b) \end{pmatrix}, \quad (H.4)$$

where the same shorthand notation for a and b is used as in Appendix G. The properties of this matrix are discussed in [133] and the determinant was computed in Appendix E:

$$\det(\mathcal{C}) = 4 \left[(a-b) \right]^{\ell} \sinh\left(\frac{\ell}{2}\operatorname{arccosh}\left(\frac{a+b}{a-b}\right) \right)^{2}.$$
 (H.5)

To find $\chi_{\ell}(k, j)$ therefore only the quadratic form of the inverse matrix in the exponent (H.3) has to be computed. Using circulant matrix properties [133] we can write $\mathcal{C}^{-1} = QD^{-1}Q^*$. Here, D is the diagonal matrix of eigenvalues $\lambda_j = 2(a+b) + 2(b-a)\cos\left(\frac{2\pi j}{\ell}\right)$ and Q is the matrix that has the eigenvectors $\mathbf{y}_j^T = \left(\rho^{j0}, \rho^{j1}, ..., \rho^{j(\ell-1)}\right)$ as columns, where $\rho = \exp\left(\frac{2\pi i}{\ell}\right)$. For expressions appearing in the first three terms of the quadratic form in (H.3) this readily yields:

$$\mathbf{u}^T \mathcal{C}^{-1} \mathbf{u} = \frac{\ell}{4b}$$
 and $\mathbf{w}_j^T \mathcal{C}^{-1} \mathbf{u} = \frac{1}{2b} \left(\tilde{a}_1 + \tilde{a}_2 \right).$ (H.6)

The computation of the last part $\boldsymbol{w}_j^T \mathcal{C}^{-1} \boldsymbol{w}_j = \boldsymbol{w}_j^T Q D^{-1} Q^* \boldsymbol{w}_j$ is slightly more involved. First we start by explicitly writing:

$$(\boldsymbol{w}_{j}^{T}Q)_{m} = (Q^{*}\boldsymbol{w}_{j})_{m}^{*} = \frac{1}{\sqrt{\ell}} \left[\left(\tilde{a}_{1} - \tilde{b}_{1} \right) + \rho^{m} \left(\tilde{a}_{1} + \tilde{b}_{1} \right) + \rho^{mj} \left(\tilde{a}_{2} - \tilde{b}_{2} \right) + \rho^{m(j+1)} \left(\tilde{a}_{2} + \tilde{b}_{2} \right) \right], \quad (\text{H.7})$$

from which follows:

$$\begin{split} \boldsymbol{w}_{j}^{T} \mathcal{C}^{-1} \boldsymbol{w}_{j} &= \\ \left(\tilde{a}_{1}^{2} + \tilde{b}_{1}^{2} + \tilde{a}_{2}^{2} + \tilde{b}_{2}^{2}\right) D_{\ell}(0) + \left(\tilde{a}_{1}^{2} - \tilde{b}_{1}^{2} + \tilde{a}_{2}^{2} - \tilde{b}_{2}^{2}\right) D_{\ell}(1) + 2 \left(\tilde{a}_{1}\tilde{a}_{2} + \tilde{b}_{1}\tilde{b}_{2}\right) D_{\ell}(j) \\ &+ (\tilde{a}_{1} - \tilde{b}_{1})(\tilde{a}_{2} + \tilde{b}_{2}) D_{\ell}(j+1) + (\tilde{a}_{1} + \tilde{b}_{1})(\tilde{a}_{2} - \tilde{b}_{2}) D_{\ell}(j-1), \end{split}$$
(H.8)

where for any $0 \le n \le \ell$:

$$D_{\ell}(n) = \frac{1}{\ell} \sum_{m=0}^{\ell-1} \frac{\rho^{mn} + \rho^{-mn}}{\lambda_m} = \frac{2}{\ell} \sum_{m=0}^{\ell-1} \frac{1}{\lambda_m \rho^{-mn}}.$$
 (H.9)

The reasoning below to compute $D_{\ell}(n)$ strongly relies on several properties of circulant matrices discussed in [139]. For any general circulant matrix $\mathcal{M} = \operatorname{circ}(c_0, c_1, \dots, c_{\ell-1})$ with eigenvalues given by [133]:

$$\lambda_m = \sum_{j=0}^{\ell-1} c_j \rho^{mj},\tag{H.10}$$

it is not difficult to see that the factors appearing in the denominator of (H.9) can be written as:

$$\lambda_m \rho^{-mn} = \sum_{j=0}^{\ell-1} c_j \rho^{m(j-n)} = c_n \rho^0 + c_{n+1} \rho^m + c_{n+2} \rho^{2m} + \dots$$
(H.11)

This is nothing else than the set of eigenvalues of a circulant matrix of which the initial row has been shifted by n to the left $P_{-n}\mathcal{M} = \operatorname{circ}(c_n, c_{n+1}, ..., c_{\ell-1}, c_0, ...)$, where P_n is defined as the circulant matrix that shifts all the rows of \mathcal{M} by one column to the right in the notation of [139]. Since circulants commute under multiplications it follows that $(P_{-n}\mathcal{M})^{-1} = P_n\mathcal{M}^{-1}$, which allows to write the summation (H.9) as:

$$D_n = \frac{2}{\ell} \operatorname{Tr} \left(P_n \mathcal{C}^{-1} \right). \tag{H.12}$$

The inverse of a three-circulant (H.4) is computed in [139]:

$$\mathcal{C}^{-1} = \operatorname{circ} \left(d_0, d_1, \dots, d_{\ell-1} \right) \tag{H.13}$$

from which follows for $0 < n \leq \ell$:

$$D_{\ell}(n) = 2d_{\ell-n}$$
 and $D_{\ell}(0) = 2d_0.$ (H.14)

Following previous assumptions that the coefficients of the circulant matrix (H.4) a and b are strictly positive with $a \neq b$, from [139] follows the following result after

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some substitutions:

$$d_{\ell-n} = \frac{1}{4\sqrt{ab}} \frac{\left(\frac{\sqrt{a}+\sqrt{b}}{\sqrt{a}-\sqrt{b}}\right)^{\ell/2-n} + \left(\frac{\sqrt{a}-\sqrt{b}}{\sqrt{a}+\sqrt{b}}\right)^{\ell/2-n}}{\left(\frac{\sqrt{a}+\sqrt{b}}{\sqrt{a}-\sqrt{b}}\right)^{\ell/2} - \left(\frac{\sqrt{a}-\sqrt{b}}{\sqrt{a}+\sqrt{b}}\right)^{\ell/2}}.$$
(H.15)

Having already cast all the expressions into a goniometric form in and Appendix G and Appendix E, we can do the same here and write:

$$D_{\ell}(n) = \frac{1}{2\sqrt{ab}} \frac{\cosh\left[\left(\frac{\ell}{2} - n\right)\operatorname{arccosh}\left(\zeta\right)\right]}{\sinh\left[\frac{\ell}{2}\operatorname{arccosh}\left(\zeta\right)\right]},\tag{H.16}$$

with $\zeta = \frac{a+b}{a-b}$. After substituting (H.5), (H.6) and (H.8) into (H.3), we can write:

$$\chi_{\ell}(k,j) = \mathcal{A}^{\ell} \sqrt{\frac{\pi^{\ell}}{4(a-b)^{\ell} \sinh\left[\frac{\ell}{2}\operatorname{arccosh}\left(\zeta\right)\right]^{2}} \exp\left(\frac{-\ell k^{2}}{16N^{2}b} - \frac{ik}{4Nb}\left(\tilde{a}_{1} + \tilde{a}_{2}\right)\right)} + \frac{1}{4}\left(\tilde{a}_{1}^{2} + \tilde{b}_{1}^{2} + \tilde{a}_{2}^{2} + \tilde{b}_{2}^{2}\right) D_{\ell}(0) + \frac{1}{4}\left(\tilde{a}_{1}^{2} - \tilde{b}_{1}^{2} + \tilde{a}_{2}^{2} - \tilde{b}_{2}^{2}\right) D_{\ell}(1) + \frac{1}{2}\left(\tilde{a}_{1}\tilde{a}_{2} + \tilde{b}_{1}\tilde{b}_{2}\right) \times D_{\ell}(j) + \frac{1}{4}(\tilde{a}_{1} - \tilde{b}_{1})(\tilde{a}_{2} + \tilde{b}_{2}) D_{\ell}(j+1) + \frac{1}{4}(\tilde{a}_{1} + \tilde{b}_{1})(\tilde{a}_{2} - \tilde{b}_{2}) D_{\ell}(j-1)\right).$$
(H.17)

To obtain the one-point cycle one has just to substitute $\tilde{a}_2 = \tilde{b}_2 = 0$ and find:

$$H_{\ell}^{(1)}(k) = \mathcal{A}^{\ell} \sqrt{\frac{\pi^{\ell}}{4(a-b)^{\ell} \sinh\left[\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right]^{2}}} \exp\left(-\frac{\ell k^{2}}{16N^{2}b} - \frac{ik\tilde{a}_{1}}{4Nb} + \frac{\tilde{a}_{1}^{2}a - \tilde{b}_{1}^{2}b}{a-b}\frac{1}{4\sqrt{ab}}\operatorname{coth}\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right) - \frac{1}{4}\frac{\tilde{a}_{1}^{2} - \tilde{b}_{1}^{2}}{a-b}\right).$$
(H.18)

The generalization to d = 3 yields the results presented in the main text in (5.29) and (5.30).

APPENDIX

Spectral decomposition of the one-particle reduced density matrix

In this appendix we will prove expression (5.44) in Chapter 5. The one-particle reduced density matrix (5.43) can be written as a summation over Gaussian states:

$$\rho_1(\mathbf{r}'|\mathbf{r}) = \frac{1}{N} \sum_{\ell=1}^N g^{(\ell)}(\mathbf{r}'|\mathbf{r}), \qquad (I.1)$$

and after rewriting the exponents in (5.43) the terms can be written as:

$$g^{(\ell)}(\mathbf{r}'|\mathbf{r}) = C\left(\frac{\gamma - \eta}{\pi}\right)^{d/2} \exp\left(-\frac{\gamma_{\ell}}{2}(\mathbf{r}^2 + \mathbf{r}'^2) + \eta_{\ell}\mathbf{r}\cdot\mathbf{r}'\right).$$
(I.2)

with:

$$C_{\ell} = \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} \frac{1}{\left|2\sinh\left(\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right)\right|^{d}}$$
(I.3)

$$\gamma_{\ell} = \frac{2m}{\beta} \sqrt{\frac{A_x}{\Delta_x}} \coth(\ell \operatorname{arccosh}(\zeta)), \qquad (I.4)$$

$$\eta_{\ell} = \frac{2m}{\beta} \sqrt{\frac{A_x}{\Delta_x}} \frac{1}{\sinh(\ell \operatorname{arccosh}(\zeta))}.$$
(I.5)

Here, the Gaussian states were suggestively written in this form to use the results from [140]. This allows to write down the solution to the Gaussian eigenvalue problem for $\mathbf{n} = (n_x, n_y, n_z)$ (in d = 3):

$$\int \mathbf{dr}' g^{(\ell)}(\mathbf{r}|\mathbf{r}')\psi_{\mathbf{n}}^{(\ell)}(\mathbf{r}') = \lambda_{\mathbf{n}}^{(\ell)}(\mathbf{r})\psi_{\mathbf{n}}^{(\ell)}$$
(I.6)

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as:

$$\lambda_{\mathbf{n}}^{(\ell)} = C_{\ell} \left(1 - \xi_{\ell} \right)^{d} \xi_{\ell}^{n_{x} + n_{y} + n_{z}},\tag{I.7}$$

$$\psi_n(\mathbf{r})^{(\ell)} = \mathcal{N}_{\mathbf{n}} H_{n_x} \left(\sqrt{\alpha_\ell} x \right) H_{n_y} \left(\sqrt{\alpha_\ell} y \right) H_{n_z} \left(\sqrt{\alpha_\ell} z \right) \exp\left(-\alpha_\ell \mathbf{r}^2 / 2 \right), \qquad (I.8)$$

with H_n a Hermite polynomial, $\alpha_{\ell} = (\gamma_{\ell}^2 - \eta_{\ell}^2)^{1/2}$, $\xi_{\ell} = \frac{\eta_{\ell}}{\gamma_{\ell} + \alpha_{\ell}}$ [140], and the normalization factor $\mathcal{N}_{\mathbf{n}} = \left(\frac{1}{2^{n_x + n_y + n_z} n_x! n_y! n_z!}\right)^{1/2} \left(\frac{\alpha_{\ell}}{\pi}\right)^{d/4}$. Remarkably, the ℓ -dependence in the coefficient α_{ℓ} drops out:

$$\alpha = \frac{2m}{\beta} \sqrt{\frac{A_x}{\Delta_x}} \left(\coth\left[\ell \operatorname{arccosh}(\zeta)\right]^2 - \frac{1}{\sinh\left[\ell \operatorname{arccosh}(\zeta)\right]^2} \right)^{1/2} = \frac{2m}{\beta} \sqrt{\frac{A_x}{\Delta_x}}.$$
(I.9)

This implies that every Gaussian state $g^{(\ell)}(\mathbf{r}'|\mathbf{r})$ has the same set of eigenstates, which are also immediately the eigenstates of (I.1):

$$\psi_{\mathbf{n}}(\mathbf{r}) = \mathcal{N}_{\mathbf{n}} H_{n_x} \left(\sqrt{\alpha} x \right) H_{n_y} \left(\sqrt{\alpha} y \right) H_{n_z} \left(\sqrt{\alpha} z \right) \exp\left(-\alpha \mathbf{r}^2 \right).$$
(I.10)

The factor ξ_ℓ does remain $\ell\text{-dependent:}$

$$\xi_{\ell} = \frac{1}{\sinh\left[\ell \operatorname{arccosh}(\zeta)\right]} \frac{1}{1 + \coth\left[\ell \operatorname{arccosh}(\zeta)\right]} = e^{-\ell \operatorname{arccosh}(\zeta)}, \quad (I.11)$$

and hence the eigenvalue of the full density matrix (I.1) corresponding to state $\psi_{\mathbf{n}}(\mathbf{r})$ is given by:

$$\lambda_{\mathbf{n}} = \frac{1}{N} \sum_{\ell=1}^{N} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} \frac{1}{\left|2\sinh\left[\frac{\ell}{2}\operatorname{arccosh}(\zeta)\right]\right|^{d}} \times \left(1 - e^{-\ell \operatorname{arccosh}(\zeta)}\right)^{d} e^{-(n_{x}+n_{y}+n_{z})\ell \operatorname{arccosh}(\zeta)}.$$
 (I.12)

In the case that $\zeta > 1$ this can be simplified even further:

$$\lambda_{\mathbf{n}} = \frac{1}{N} \sum_{\ell=1}^{N} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} e^{-\left(\frac{1}{2} + n_x + n_y + n_z\right)\ell \operatorname{arccosh}(\zeta)}.$$
 (I.13)

APPENDIX **U**

The Bogoliubov-Fröhlich model at zero temperature

In this appendix we will argue that in the context of our bosonic variational models the expectation value of the effective polaron action of the Bogoliubov-Fröhlich model $\langle S_{\text{eff}} \rangle$ can be computed as if the impurities are distinguishable. We start by noting that for the Bogoliubov-Fröhlich model, regardless of β -periodicity of the expectation values, the remaining quantity of interest required to obtain the variational free energy (6.22) is given by:

$$\Gamma_{\mathbf{k}} = \frac{1}{\hbar\beta} \int_{0}^{\hbar\beta} d\tau \int_{0}^{\hbar\beta} d\sigma \mathcal{G}_{\mathbf{k}} \left(\tau - \sigma\right) \mathcal{F}_{\mathbf{k}} \left(\tau, \sigma\right) \tag{J.1}$$

with:

$$\mathcal{F}_{\mathbf{k}}(\tau,\sigma) = \langle \rho_{\mathbf{k}}(\tau_1)\rho_{\mathbf{k}}^*(\sigma) \rangle = N\mathcal{F}_{\mathbf{k}}^{(1)}(\tau,\sigma) + N(N-1)\mathcal{F}_{\mathbf{k}}^{(2)}(\tau,\sigma), \qquad (J.2)$$

and:

$$\mathcal{F}_{\mathbf{k}}^{(1)}(\tau,\sigma) = \left\langle e^{i\mathbf{k}[\mathbf{r}_{i}(\tau)-\mathbf{r}_{i}(\sigma)]} \right\rangle,\tag{J.3}$$

$$\mathcal{F}_{\mathbf{k}}^{(2)}(\tau,\sigma) = \left\langle e^{i\mathbf{k}[\mathbf{r}_{i}(\tau) - \mathbf{r}_{j}(\sigma)]} \right\rangle \quad \text{for} \quad i \neq j.$$
(J.4)

We have already learned to derive these type of two-point correlation functions with respect to the bosonic model system in expression (5.32) of Chapter 5 for a general source function. Applying the formalism to specifically (J.3) and (J.4) we Chapter J - The Bogoliubov-Fröhlich model at zero temperature

obtain:

$$\mathcal{F}_{\mathbf{k}}^{(1)}(\tau,\sigma) = \frac{1}{N} \sum_{\ell=1}^{N} \frac{1}{\left[2\sinh\left(\frac{\ell}{2}q\right)\right]^d} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} \exp\left(-\frac{k^2}{4m}\left(\varphi_1(\tau-\sigma)+\varphi_2(\tau,\sigma)\right)\right),\tag{J.5}$$

$$\mathcal{F}_{\mathbf{k}}^{(2)}(\tau,\sigma) = \frac{1}{N(N-1)} \sum_{\ell=2}^{N} \frac{1}{\left[2\sinh\left(\frac{\ell}{2}q\right)\right]^{d}} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)}$$
$$\times \sum_{j=1}^{\ell-1} \left[\frac{h_{j}(\mathbf{0})h_{\ell-j}(\mathbf{0})}{h_{\ell}(\mathbf{0})} \times \exp\left(-\frac{k^{2}}{4m}\xi_{1}\right) + \exp\left(-\frac{k^{2}}{4m}\xi_{2}\right)\right]. \tag{J.6}$$

The exponents are given by:

$$\varphi_{1}(\tau - \sigma) = \frac{1}{N} \left[(N - 1)(D_{x}(0) - D_{x}(\tau - \sigma)) + D_{y}(0) - D_{y}(\tau - \sigma) \right], \quad (J.7)$$

$$\varphi_{2}(\tau, \sigma) = \frac{1}{2} \frac{1}{1 - B_{x}D_{x}} \left[B_{x} \left(D_{x}(\tau) - D_{x}(\sigma) \right)^{2} - D_{x} \left(\delta_{x}(\tau) - \delta_{x}(\sigma) \right)^{2} \right]$$

$$\times \left(1 - \frac{1}{\sqrt{B_{x}D_{x}}} \operatorname{coth}\left(\frac{\ell}{2}q\right) \right). \quad (J.8)$$

and

Here, we have also redefined the notation of the J-factors (5.36) introduced Chapter 5:

$$I_1(\tau) = \beta J_1(\tau) = \frac{1}{B_x D_x - 1} \left[B_x D_x(\tau)^2 - D_x \delta_x(\tau)^2 \right],$$

$$I_2(\tau, \sigma) = \beta J_2(\tau, \sigma) = \frac{1}{B_x D_x - 1} \left[B_x D_x(\tau) D_x(\sigma) - D_x \delta_x(\tau) \delta_x(\sigma) \right],$$

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$$I_3(\tau,\sigma) = \beta X(\tau,\sigma) = \frac{1}{B_x D_x - 1} \left[D_x(\tau) \delta_x(\sigma) - D_x(\sigma) \delta_x(\tau) \right].$$

where functions Δ_x , A_x and $\partial_{\tau} \Delta_x(\tau)$ are given by:

$$D_x(u) = \beta \Delta_x(u) = \beta \frac{4}{\beta^2} \sum_{n=-\infty}^{\infty} \frac{e^{i\nu_n u}}{\nu_n^2 + x_n},$$
$$B_x = \frac{1}{\beta} A_x = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{x_n}{\nu_n^2 + x_n},$$
$$\delta_x(u) = \frac{\beta}{2} \partial_\tau \Delta_x(\tau) = \frac{2}{\beta} \sum_{n=-\infty}^{\infty} \frac{i\nu_n e^{i\nu_n u}}{\nu_n^2 + x_n},$$

and where we use the shorthand notation $D_x(0) = D_x$. In addition we have introduced the following shorthand notation for the argument of the hyperbolic sine in (J.5) and (J.6) as:

$$q = \operatorname{arccosh}\left[\frac{A_x \Delta_x + 1}{A_x \Delta_x - 1}\right]).$$
(J.11)

Next, we proceed to discuss the behavior of $\Gamma_{\mathbf{k}}$ in the zero temperature limit. However, a major obstacle in doing this is that the function $\mathcal{F}_{\mathbf{k}}(\tau,\sigma)$ is not strictly dependent on $u = \tau - \sigma$, but also depends on $\tau + \sigma$, and hence some care should be taken with the typical symmetry arguments as used for a single impurity. Indeed, the arguments in the exponentials: φ_2 , ξ_1 and ξ_2 do have some explicit τ and σ -dependence. To deal with this problem, first we define the integrand of (J.1) function:

$$I_{\Gamma}(\tau,\sigma) = \mathcal{G}_{\mathbf{k}}(u) \mathcal{F}_{\mathbf{k}}(\tau,\sigma). \qquad (J.12)$$

It is not too difficult to show, using the symmetries of the functions $D_x(u)$ and $\delta_x(u)$ that without any loss of generality, after transforming to relative $u = \tau - \sigma$ and center of mass coordinates $Q = (\tau + \sigma)/2$ the integral (J.1) can be written as:

$$\Gamma_{\mathbf{k}} = \frac{4}{\beta} \int_{0}^{\frac{\beta}{2}} du \left[\int_{\frac{u}{2}}^{\frac{\beta}{2}} dQ \ I_{\Gamma} \left[Q + \frac{u}{2}, Q - \frac{u}{2} \right] + \int_{0}^{\frac{u}{2}} dQ \ I_{\Gamma} \left[Q + \frac{u}{2}, Q - \frac{u}{2} \right] \right]. \tag{J.13}$$

We should now make the crucial observation that in the limit of $\beta \to \infty$ only the section of this integral that diverges as $\sim \beta$ provides a non-vanishing contribution to $\Gamma_{\mathbf{k}}$, which significantly simplifies the approach in this limit. In (J.13) we have already exploited the symmetries in the integrand to fold the parts where $u > \beta/2$

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onto themselves, which allows us to write without loss of generality:

$$\lim_{\beta \to \infty} I_{\Gamma}(\tau, \sigma) = e^{-\omega_{\mathbf{k}} u} \left\langle \rho_{\mathbf{k}}(\tau_1) \rho_{\mathbf{k}}^*(\sigma) \right\rangle.$$
 (J.14)

The triangle inequality can now be used to notice that the absolute value of $\langle \rho_{\mathbf{k}}(\tau_1) \rho_{\mathbf{k}}^*(\sigma) \rangle$ is bounded by N_I^2 and hence for any value of Q the integrand to goes to zero exponentially fast:

$$\lim_{\beta \to \infty} \lim_{u \to \beta/2} I_{\Gamma}(\tau, \sigma) = 0 \tag{J.15}$$

It naturally follows from this argument that the integrand of the second term in (J.13) goes to zero much faster than the growth of the integration domain as u increases and hence:

$$\Gamma_{\mathbf{k}} = \frac{4}{\beta} \int_0^{\frac{\beta}{2}} du \int_{\frac{u}{2}}^{\frac{\beta}{2}} dQ \ I_{\Gamma} \left[Q + \frac{u}{2}, Q - \frac{u}{2} \right].$$
(J.16)

Combining all of the previous observations, it appears that the $\sim \beta$ divergence in the integral has to arise due to I_{Γ} going to finite value as Q becomes large:

$$\frac{1}{\beta} \int_{\frac{u}{2}}^{\frac{\beta}{2}} dQ \ I_{\Gamma} \left[Q + \frac{u}{2}, Q - \frac{u}{2} \right] = \frac{1}{2} \lim_{Q \to \infty} I_{\Gamma} \left[Q + \frac{u}{2}, Q - \frac{u}{2} \right] + \mathcal{O} \left(\beta^{-1} \right), \quad (J.17)$$

which would allow us to write:

$$\Gamma_{\mathbf{k}} = 2 \lim_{Q \to \infty} \int_0^{\frac{\beta}{2}} du \ I_{\Gamma} \left[Q + \frac{u}{2}, Q - \frac{u}{2} \right]. \tag{J.18}$$

Let us now confirm this and discuss this limit more carefully. From expressions (J.5) and (J.6) we can see that the large Q limit will be determined by the behavior of the four arguments of the exponential functions φ_1 , φ_2 , ξ_1 and ξ_2 . Since φ_1 only depends explicitly on u, it remains unchanged in this limit. For $\varphi_2(\tau, \sigma)$, we can observe that in the presence of a non-constant memory kernel $x_n \neq \text{cst}$, the factors $1 - B_x D_x$ and $\left(1 - \frac{1}{\sqrt{B_x D_x}} \coth\left(\frac{\ell}{2}q\right)\right)$ remain finite in the temperature zero limit and hence what concerns the limiting behavior of φ_2 we can write:

$$\lim_{\beta \to \infty} \varphi_2(\tau, \sigma)$$
= finite non-zero factor × $\left[B_x \left(D_x(\tau) - D_x(\sigma) \right)^2 - D_x \left(\delta_x(\tau) - \delta_x(\sigma) \right)^2 \right].$
(J.19)

Both $D_x(\tau)$ and $\delta_x(\tau)$ go to zero for large $\tau < \beta/2$. For example, for the toy model system we considered in Chapters 4 and 5, one can readily confirm that at low temperatures:

$$D_x(\tau) = \frac{2\gamma_+}{\omega_+} e^{-\omega_+\tau} + \frac{2\gamma_-}{\omega_-} e^{-\omega_-\tau},$$

$$\delta_x(\tau) = -\left[\gamma_+ e^{-\omega_+\tau} + \gamma_- e^{-\omega_-\tau}\right].$$

At the same time we remember that in the integral (J.16) the large u behavior is exponentially damped and while taking the $Q \to \infty$ limit we can just as well assume that $u \ll \beta/2$. This regime of course corresponds to both τ and σ being simultaneously large since $\tau = Q + \frac{u}{2}$ and $\sigma = Q - \frac{u}{2}$ from which follows that φ_2 goes to zero in this limit. Through similar arguments the terms with explicit dependence on τ and σ in ξ_1 and ξ_2 vanish such that:

$$\xi(\tau - \sigma) = \xi_1 = \xi_2 = \frac{1}{N_I} \left[(N_I - 1)D_x + D_y + D_x(\tau - \sigma) - D_y(\tau - \sigma) \right].$$
(J.20)

We can now write:

$$\begin{aligned} \mathcal{F}_{\mathbf{k}}^{(1)}(\tau,\sigma) &= \frac{1}{N} \sum_{\ell=1}^{N} \frac{1}{\left[2\sinh\left(\frac{\ell}{2}q\right)\right]^{d}} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} \exp\left(-\frac{k^{2}}{4m}\varphi(\tau-\sigma)\right), \quad (J.21) \\ \mathcal{F}_{\mathbf{k}}^{(2)}(\tau,\sigma) &= \frac{1}{N(N-1)} \sum_{\ell=2}^{N} \frac{1}{\left[2\sinh\left(\frac{\ell}{2}q\right)\right]^{d}} \frac{\mathbb{Z}(N-\ell)}{\mathbb{Z}(N)} \exp\left(-\frac{k^{2}}{4m}\xi(\tau-\sigma)\right) \\ &\times \sum_{j=1}^{\ell-1} \left[\frac{h_{j}(\mathbf{0})h_{\ell-j}(\mathbf{0})}{h_{\ell}(\mathbf{0})} + 1\right]. \end{aligned}$$
(J.22)

The remaining exponents no longer depend on the cyclic indicies ℓ and j and hence can be taken outside of the summations. From (5.17) readily follows that:

$$\frac{1}{N_I} \sum_{\ell=1}^{N_I} \frac{1}{\left[2\sinh\left(\frac{\ell}{2}q\right)\right]^d} \frac{\mathbb{Z}(N_I - \ell)}{\mathbb{Z}(N_I)} = 1$$
(J.23)

We can also use the following result from [108]:

$$\sum_{\ell=2}^{N_I} \frac{1}{\left[2\sinh\left(\frac{\ell}{2}q\right)\right]^d} \frac{\mathbb{Z}(N_I - \ell)}{\mathbb{Z}(N_I)} \sum_{j=1}^{\ell-1} \left[\frac{h_j(\mathbf{0})h_{\ell-j}(\mathbf{0})}{h_\ell(\mathbf{0})} + 1\right] = (N_I - 1)N_I. \quad (J.24)$$

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The functions (J.21) and (J.22) simplify significantly to:

$$\mathcal{F}_{\mathbf{k}}^{(1)}(\tau,\sigma) = \exp\left(-\frac{k^2}{4m}\varphi(\tau-\sigma)\right),\tag{J.25}$$

$$\mathcal{F}_{\mathbf{k}}^{(2)}(\tau,\sigma) = \exp\left(-\frac{k^2}{4m}\xi(\tau-\sigma)\right),\tag{J.26}$$

which can be readily shown to be nothing else than the result for distinguishable particles.

Academic curriculum vitae

List of publications

- N. Verhelst, T. Ichmoukhamedov, J. Tempere, "Radial vortex core oscillations in Bose-Einstein condensates", The European Physical Journal Special Topics, 226, 2829–2836 (2017).
- T. Ichmoukhamedov, J. Tempere, "Feynman path-integral treatment of the Bose polaron beyond the Fröhlich model", Phys. Rev. A **100**, 043605 (2019).
- T. Ichmoukhamedov, J. Tempere, "Vortices in Fermi gases with spin-dependent rotation potentials", Phys. Rev. A **101**, 053609 (2020)
- T. Ichmoukhamedov, J. Tempere, "Path-integral approach to the thermodynamics of bosons with memory: Partition function and specific heat" Phys. Rev. A **104**, 023322 (2021)
- T. Ichmoukhamedov, J. Tempere, "Path-integral approach to the thermodynamics of bosons with memory: Density and correlation functions", Phys. Rev. A **104**, 062201 (2021)
- T. Ichmoukhamedov, J. Tempere, "General memory kernels and further corrections to the variational path integral approach for the Bogoliubov-Fröhlich Hamiltonian", Phys. Rev. B 105, 104304 (2022)

Grants and projects

PhD fellowship: FWO (Fonds Wetenschappelijk Onderzoek - Vlaanderen) Fundamental Research predoctoral fellowship 2018-2022 - project: "Many-polaron effects in a Bose-Einstein condensate", Project numbers: 1135519N and 1135521N.

Conferences and workshops

- Poster presentation Feynman path-integral treatment of the Bose polaron beyond the Fröhlich model, at the workshop: Compound (Atomic) Quantum Systems Leiden, Netherlands (2019)
- Poster presentation *Feynman path-integral treatment of the Bose polaron beyond the Fröhlich model* at the conference: Theory at Sea - Oostende, Belgium (2019)
- Attended summer school: *Methods of Path Integration in Modern Physics* Bad Honnef, Germany (2019)

Chapter J - The Bogoliubov-Fröhlich model at zero temperature

- Poster presentation Feynman path-integral treatment of the Bose polaron beyond the Fröhlich model, at the workshop: Polarons in the 21st Century Vienna, Austria (2019)
- Poster presentation *Path integral description of bosons with memory* at conference: Quantum Fluids and Solids conference - originally: Bangalore, India (online due to COVID) (2021)
- Talk on 5/05/22: Path integral description of quadratic systems with general memory, at the Belgian Quantum Physics Initiative meeting, Brussels, Belgium (2022)

Teaching assistant

- Path Integrals for Option Pricing 2018-2019
- Path Integrals for Quantum Mechanics 2019-2020
- Quantum Field Theory 2019-2020
- Path Integrals for Option Pricing 2020-2021
- Quantum Mechanics 2020-2021
- Path Integrals for Quantum Mechanics 2021-2022
- Quantum Mechanics 2021-2022

Outreach efforts

- Coorganizing and hosting an educational show "Koud, kouder, koudst" at our lab (2019).
- Supervising and guiding high school interns with their projects at our research group (2019).
- Participated in the "Children's University" outreach event of the University of Antwerp aimed at getting young children interested in science (2019).
- Former member of the Qcraft/Elementarycraft projects (2019-2021) of the University of Antwerp, where I have participated in developing an educational Minecraft mod.
- Hosting a Qcraft workshop at the "Day of Science at the Beacon" event in Antwerp (2019).
- Hosting a Qcraft workshop for the studio STEM "Proefkot" event at the University of Antwerp (2019).
- Hosting a workshop table at the popular University of Antwerp "Fusion Show" visited by hundreds of high schools in Antwerp (2021).

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