

Faculteit Wetenschappen Departement Fysica Theorie van Kwantumsystemen en Complexe Systemen

A treatise on Wigner distributions: from particles and polarons to fields

Over Wigner verdelingsfuncties: van deeltjes en polaronen tot velden

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The elements of the behavior which are not specified by the laws of nature are called initial conditions. These, then, together with the laws of nature, specify the behavior as far as it can be specified at all.

EUGENE P. WIGNER, Nobel Lecture, 1963

Preface

My journey towards this work and to the subject of theoretical condensed matter physics in general, has been somewhat unconventional. In the context of this work I would say it can not accurately be described by the classical trajectory. As an electronic device engineer and master of nanoscience my primary interest lay in the optimization and design of nano-CMOS transistors. However, after graduating from the KULeuven I moved to the *"Theory of quantum and complex systems"* group at the University of Antwerp to start my PhD; my first jump. As with all transitions, it came with a certain degree of unpleasantness. Whereas I had left my engineering career in a quest for a more profound, rigorous, knowledge of the laws of physics, I suddenly found myself in a place where rigor seemed to be far beyond my capability. However, I soon found out that most problems were caused by a certain language problem. To give an example; I would never have understood the phrase "*The grand partition function is the generating function of the canonical partition function*" but it would almost be self evident that the former is usually much easier to find when stating that "*The grand partition function is the z-transform of the canonical partition function*".

At my arrival, Prof. dr. Fons Brosens showed me some of the ideas and results he had obtained on aspects of time reversal symmetry using the concept of Wigner distributions. Impressed by the results, I extended and refined some of these methods and this has become the content of my PhD thesis.

This work would not have been possible without the help and support of Fons Brosens. Thank you Fons, for not telling me what to do and giving me the opportunity and freedom to develop my research in a direction which I deemed best. Thank you for the many interesting discussions. I hope you enjoyed them as much as I did.

I would also like to thank my other promotor Prof. dr. Jacques Tempere for comments and suggestions on my work. Furthermore, I thank Prof. dr. W. Magnus for many useful discussion and for the pleasant collaboration, in particular on the content of chapter 2.

I am also indebted to Prof. dr. J.T. Devreese for introducing me to the polaron problem. I greatly benefited from our weekly discussion on polarons. It is during these discussions that I learned about the infamous 3/2kT problem and various sum rules which now form an indispensable part of this work. I furthermore acknowledge valuable work notes by Devreese and Klimin.

I sincerely thank all the members of my jury, in particular Prof. dr. Hagen Kleinert, Prof. dr. Anatoli Polkovnikov and Prof. dr. Lawrence Schulman, for useful comments on the manuscript and suggestions for future research.

Finally, I would like to take this opportunity to thank my family and friends for their support, encouragements and unconditional love. Above all, I thank Sien for her inexhaustible patience, for sleeping on the sofa while I finish my calculations. For simply accepting me as I am.

Dries Sels Antwerp, May 6, 2014

Excerpt

In dit werk onderzoeken we Wigners faseruimte formulering van de kwantummechanica. We baseren ons hierbij vooral op Feynmans Lagrangiaanse of padintegraal beschrijving van de kwantummechanica. In tegenstelling tot de Hamiltoniaanse beschrijving wordt het gebruik van operator vermeden in zowel Feynmans als Wigners formulering van de theorie. Beide methodes delen bovendien hun affiniteit met de klassieke mechanica. De relatie tussen de klassieke en de kwantum mechanica is dan ook een wederkerend thema in dit werk. Wigners formulering dankt zijn aantrekkingskracht vooral aan de gelijkenis met de klassieke statistische mechanica. Als gevolg van Heisenbergs onzekerheidsrelatie bezet zelfs één deeltje een minimaal volume in de faseruimte. Het is daarom aanlokkelijk om een analogie te zoeken tussen de klassieke statistische fluctuaties in een ensemble van klassieke deeltjes en de kwantumfluctuaties van één kwantumdeeltje. De verandering van de klassieke beweging door kwantumfluctuaties is echter precies de intuïtieve interpretatie van Feynmans padintegraal beschrijving van het probleem. Verschillende aspecten van het kwantum-klassieke correspondentieprincipe worden beschouwd. In het bijzonder bestuderen we de klassieke limiet in (i) één deeltjes systemen, (ii) systemen in interactie met de buitenwereld, (iii) bosonische kwantumvelden.

Hoofdstuk 2 introduceert de Wigner functie voor een ééndeeltjessysteem. Een elementaire introductie tot Weyl ordening en Bopp operatoren wordt gegeven. Vervolgens ligt de focus op de evolutie van een initiële toestand in de tijd. De propagator voor de Wignerverdeling wordt afgeleid uit Feynmans padintegraal en we tonen aan dat het resultaat equivalent is met de oplossing van Von Neumann's vergelijking voor de dichtheidsmatrix. Voorts bevat hoodstuk 2 een analytische behandeling van de harmonische oscillator en het tweespletenexperiment. Voor de harmonische oscillator vinden we het gekende resultaat dat de klassieke en de kwantum dynamica identiek is. De combinatie van padintegralen met Wignerfuncties biedt bovendien een bijzonder intuïtieve verklaring voor het tweespletenexperiment.

Tenslotte bestuderen we, in detail, de semi-klassieke *truncated* Wigner benadering. De volledige kwantumdynamcia wordt ontwikkeld in kwantumsprongen rond het klassieke pad. Binnen de *truncated* Wigner benadering negeren we het effect van de kwantumsprongen. We benaderen dus de kwantumdynamica door de klassieke evolutie van het systeem. Deze benadering wordt gerechtvaardigd door het feit dat elke kwantumsprong een extra gewicht \hbar^2 toevoegt aan het pad. De convergentie van deze ogenschijnlijke expansie in \hbar hangt echter sterk af van de Hamiltoniaan en de toestand van het systeem. De Moyal expansie bevat immers steeds hogere afgeleiden van beiden. Als alternatief stellen we daarom een *variatonele truncated* Wigner benadering voor. De methode expandeert de volledige kwantumdynamica rond een fictieve klassieke evolutie, rond dewelke het effect van kwantumfluctuaties minimaal is.

In hoofdstuk 3 breiden we het resultaat uit naar gekoppelde systemen. In vele gevallen is slechts een deel van het systeem fysisch toegankelijk of relevant. We stellen daarom de propagator voor de gereduceerde of marginale Wignerverdeling van het relevante systeem op. We focussen hierbij op een deeltje gekoppeld met een set van harmonisch oscillatoren. Zolang de koppeling tussen beiden bilineair is blijft het geheel analytisch behandelbaar. Als voorbeeld werken we de Ohmse Caleira-Leggett propagator uit en presenteren we de lineaire respons coëfficiënten voor niet Ohmse warmtebaden. Vervolgens spitsen we de aandacht toe op het polaron probleem. Als gevolg van de niet-lineaire koppeling tussen het systeem en het bosonisch bad kunnen we hierbij niet analytisch te werk gaan. We ontwikkelen een perturbatietheorie en leiden daaruit de bewegingsvergelijking voor het gereduceerde systeem af. We tonen aan onder welke omstandigheden de gereduceerde Liouville vergelijking voldoet aan de lineaire Wigner-Boltzmann vergelijking. Tenslotte presenteren we een alternatieve methode om de lineaire respons coëfficiënten van het gekoppeld systeem te berekenen. De methode is gebaseerd op een systematische expansie van de kwantum Liouville vergelijking.

Hoofdstuk 4 beschrijft tenslotte de veralgemening van de resultaten voor het ééndeeltjessysteem naar een (veeldeeltjes) kwantumveld. In overeenkomst met de resultaten in hoofdstuk 2 vinden we dat voor alle harmonische problemen alleen het klassieke pad bijdraagt tot de propagator. De klassieke bewegingsvergelijking is in dit geval echter de Schrödinger vergelijking voor het veld in plaats van de Newtoniaanse bewegingsvergelijking voor het deeltje uit hoofdstuk 2. Voor niet kwadratische, interagerende problemen zijn we wederom aangewezen op een benaderende behandeling. We veralgemenen de voorgaande analyse en presenten een stochastische differentiaalvergelijking voor het kwantumveld. Het effect van de kwantumruis op het systeem hangt sterk af van de initiële toestand. We passen daarom de *variatonele truncated* Wigner benadering toe op een volledig coherente toestand en verklaren het verschil met de semi-klassieke *truncated* Wigner benadering.

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Chapter 1

Introduction

Since the seminal work by Wigner [1] phase space methods have attracted intense theoretical attention. The interest in phase space methods has only increased over the years and it has found important applications in the fields of quantum optics [2, 3, 4], atomic physics [5], cold atoms [6] or other bosonic systems [7,8]. Also in quantum transport theory Wigner's distribution function has been investigated as a tool to propagate the signatures of quantum statistics into the time-dependent solution [9,10,11]. In quantum transport the method provides an alternative to the non-equilibrium Keldysh-Schwinger [12,13] Green's function method. Although both methods are formulated in a completely different language they provide equivalent information about the dynamics of quantum systems. In fact the connection between the Wigner distribution and the Keldysh Green function was first provided by Kadanoff and Baym [14].

Wigner's formulation of quantum mechanics is attractive because of its similarity to classical statistical mechanics. Due to Heisenberg's uncertainty principle even a single particle occupies a minimal area in phase space. Consequently it's appealing to consider the correspondence between classical statistical fluctuations in an ensemble of particles and quantum fluctuations of a single particle in phase space. Significant theoretical effort has thus been put into the investigation of the semiclassical dynamics [15, 16, 7] of the Wigner distribution.

As an alternative to the Hamiltonian description of quantum mechanics one may adopt Feynman's Lagrangian formulation of quantum mechanics [17]. This approach essentially relies on the calculation of the Green function or propagator appearing as a path integral, rather than on solving the dynamic equations for the density matrix. Moreover, Feynman's approach also exhibits a direct link to classical mechanics through the explicit occurrence of the classical action in the path integral. In fact the modification of classical mechanics by quantum fluctuations is precisely the intuitive understanding of Feynman's path integral description of quantum mechanics. By adopting a saddle-point expansion [18] ones can for example derive the semiclassical Van Vleck-Gutzwiller propagator [19, 20, 21]. By construction, the quantum fluctuations around the Euler-Lagrange equations associated with the saddle-point are minimal.

The primary goal of this work is to discuss, in detail, the Lagrangian approach to Wigner's phase space formulation of quantum mechanics. For readers unfamiliar with the Lagrangian formulation of quantum mechanics I recommend to consult one of the following standard works [17, 18, 22, 23]. I include the original work [17] by Feynman as it is of remarkable clarity.

The work is divided into three parts. In chapter 2 we discuss the time evolution of a single particle system in phase space. After formally introducing the Wigner function in section 2.1, the propagator is derived within the path integral description of quantum mechanics in section 2.2. Next we discuss two important yet analytically tractable examples, i.e. the harmonic oscillator and the double slit experiment. The remaining part of chapter 2 is devoted to a discussion of semiclassical approximations to the Wigner propagator.

In chapter 3 we extend the obtained result by computing the path integral for the propagator

of the reduced Wigner function of a system coupled to an external quantum system. This extension may be seen as the Wigner–Weyl formulation of the theory of influence functionals developed by Feynman and Vernon [24]. Although this can be done for arbitrary systems we again focus on a single particle interacting with some bath. The general results are derived in section 3.1. In section 3.2 the focus lies on a particle connected to a set of harmonic oscillator such that the dynamics of the bath is analytically tractable. As a fully solvable example we discuss the Caldeira-Leggett model [25]. The remaining part of chapter 3 is devoted to a discussion of the polaron, a quasi-particle formed trough the interaction of the real particle with the bath. Due to the non-linearity of the coupling between the system and the bosonic bath, the dynamics can not be solved analytically. An approximate solution for the linear response coefficient is presented in section 3.4, based on the perturbation theory developed in section 3.3.

Chapter 4 is concerned with a second quantized description of the Wigner distribution and its propagation in time. We thus generalize the results presented in chapter 2 from a single particle to a complete field. The discussion is limited to bosonic quantum field theories. Using the language developed in section 2.4 we, once again, discuss semiclassical approximation of the exact Wigner propagator for the quantum field theory.

Concluding remarks, an outline for further research and an overview of the author's scientific contributions can be found in chapter 5.

Chapter 2

Single particle Wigner distribution

This chapter is concerned with a first quantized description of the Wigner function and with its propagation in time. For notational simplicity, but without loss of generality, the presentation is restricted to a single particle moving in one dimension. After introducing the Wigner function in section 2.1, we derive the propagator within Feynman's Lagrangian description of quantum mechanics in section 2.2. Explicit solutions are provided for solvable problems such as the harmonic oscillator and the double-slit experiment, the latter is rather difficult to explain within the Hamiltonian formulation of the problem. In the final section 2.4 we discuss different approximations for situations in which the path integral can not be solved exactly. Considerable attention is devoted to the semiclassical limit.

2.1 The Wigner distribution

The Wigner distribution function [1] f(x, p) associated with state characterized by a density matrix $\hat{\rho}$ is defined as

$$f(x,p) = \int \left\langle x + \frac{\xi}{2} \right| \hat{\rho} \left| x - \frac{\xi}{2} \right\rangle \exp\left(-\frac{i}{\hbar}p\xi\right) \frac{\mathrm{d}\xi}{2\pi\hbar}$$
(2.1)

$$= \int \left\langle p + \frac{\kappa}{2} \right| \hat{\rho} \left| p - \frac{\kappa}{2} \right\rangle \exp\left(\frac{i}{\hbar} x \kappa\right) \frac{\mathrm{d}\kappa}{2\pi\hbar}, \qquad (2.2)$$

where $|x\rangle$ and $|p\rangle$ are position and momentum eigenstates respectively. To quote Wigner, one can *call* f(x, p) the probability function of the simultaneous values of x for the coordinate and p for the momentum. It has the important property that the correct marginal probabilities are recovered when integrated over one of the two conjugate variables

$$n(x) = \int f(x, p) dp = \langle x | \hat{\rho} | x \rangle,$$

$$n(p) = \int f(x, p) dx = \langle p | \hat{\rho} | p \rangle,$$

which suggests it is indeed the joint probability distribution of x and p. As already noted by Wigner himself the function is real but not necessarily positive. The Wigner function can therefore not be a true probability distribution but it belongs to a class of quasi-probability distributions. Many such distributions exist in quantum mechanics but of all of them, the Wigner distribution is the only one to have the correct marginal distributions [4]. It is moreover easy to show from the definition that the expectation value of any operator \hat{A} can be calculated as a classical average over phase space

$$\left\langle \hat{A} \right\rangle = \operatorname{Tr}\left[\hat{A}\hat{\rho}\right] = \iint A(x,p)f(x,p)\mathrm{d}p\mathrm{d}x,$$
(2.3)

if A(x, p) is given by

$$A(x,p) = \int \left\langle x + \frac{\xi}{2} \right| \hat{A} \left| x - \frac{\xi}{2} \right\rangle \exp\left(-\frac{i}{\hbar}p\xi\right) d\xi, \qquad (2.4)$$

$$= \int \left\langle p + \frac{\kappa}{2} \left| \hat{A} \right| p - \frac{\kappa}{2} \right\rangle \exp\left(\frac{i}{\hbar} x \kappa\right) d\kappa.$$
 (2.5)

The function A(x, p) is usually called the Weyl-representation of the operator \hat{A} . It follows from the previous expression that the Weyl-representations A(x) and A(p) of operators $A(\hat{x})$ and $A(\hat{p})$ that commute with \hat{x} and \hat{p} respectively can simply be found by replacing the operators by ordinary numbers. Note that this was already implied by the fact that the Wigner function has the correct marginal distributions. In general one has to evaluate expression (2.4) or (2.5) to obtain the Weyl-representation of an operator. Consider for example $\hat{A} = \hat{x}\hat{B}$, where \hat{B} does not neccessarily commute with \hat{x} . Using (2.4) we find

$$A(x,p) = \int \left(x + \frac{\xi}{2}\right) \left\langle x + \frac{\xi}{2} \middle| \hat{B} \middle| x - \frac{\xi}{2} \right\rangle \exp\left(-\frac{i}{\hbar}p\xi\right) d\xi$$
$$= \left(x + \frac{i\hbar}{2}\frac{\partial}{\partial p}\right) B(x,p).$$

The same analysis can be done for an operator $\hat{A} = \hat{p}\hat{B}$. This time using (2.5), we find

$$A(x,p) = \int \left(p + \frac{\kappa}{2}\right) \left\langle p + \frac{\kappa}{2} \left| \hat{B} \right| p - \frac{\kappa}{2} \right\rangle \exp\left(\frac{i}{\hbar}x\kappa\right) d\kappa$$
$$= \left(p - \frac{i\hbar}{2}\frac{\partial}{\partial x}\right) B(x,p).$$

One can actually repeat this procedure over and over again [26], and eventually take \hat{B} to be the identity operator. According to this prescription the Weyl-representation A(x, p) of an operator \hat{A} can be constructed by replacing position and momentum operators by

$$\hat{x} \to x + \frac{i\hbar}{2} \frac{\partial}{\partial p} \text{ and } \hat{p} \to p - \frac{i\hbar}{2} \frac{\partial}{\partial x}.$$
 (2.6)

These operators are usually called Bopp operators. Note that they indeed satisfy canonical commutation relations. Instead of working in the x or p representation where the conjugate variable becomes a derivative, the present representation is more symmetric. The Weyl-representation is therefore also called the symmetric representation.

2.2 Single-particle phase space propagator

Consider a single-particle system, in one dimension, whose generalized coordinate is denoted by x. The quantum-mechanical amplitude for the system to go from position x_a at time $t = t_a$ to position x_b at time $t = t_b$ is given by the Feynman path integral

$$K(x_b, t_b | x_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x(t) \exp\left(\frac{i}{\hbar} S[x(t)]\right), \qquad (2.7)$$

where S[x(t)] is the action of the system for a trajectory x(t). Let $\{|n\rangle\}$ denote a complete orthonormal set of states. The amplitude $A(n_b, t_b|n_a, t_a)$ for being in state $|n_b\rangle$ at time t_b , if initially in state $|n_a\rangle$ at time t_a , is then given by

$$A(n_b, t_b | n_a, t_a) = \iint \langle n_b | x_b \rangle K(x_b, t_b | x_a, t_a) \langle x_a | n_a \rangle dx_a dx_b.$$
(2.8)

The corresponding transition probability $P(n_b, t_b | n_a, t_a) = |A(n_b, t_b | n_a, t_a)|^2$ can thus be written as

$$P(n_b, t_b | n_a, t_a) = \iiint \langle x'_b | n_b \rangle \langle n_b | x_b \rangle K^*(x'_b, t_b | x'_a, t_a) K(x_b, t_b | x_a, t_a) \times \langle x_a | n_a \rangle \langle n_a | x'_a \rangle dx_a dx_b dx'_a dx'_b.$$
(2.9)

The total probability to be in state $|n_b\rangle$ at $t = t_b$ is the sum over all possible transitions from $|n_a\rangle$ to $|n_b\rangle$, weighted by the initial probability to be in a given state $|n_a\rangle$:

$$P(n_b, t_b) = \sum_{n_a} P(n_a, t_a) P(n_b, t_b | n_a, t_a), \qquad (2.10)$$

Substituting (2.9) in (2.10) leads to

$$P(n_b, t_b) = \iiint \langle x'_b | n_b \rangle \langle n_b | x_b \rangle K^*(x'_b, t_b | x'_a, t_a) K(x_b, t_b | x_a, t_a) \times \left\{ \sum_{n_a} P(n_a, t_a) \langle x_a | n_a \rangle \langle n_a | x'_a \rangle \right\} dx_a dx_b dx'_a dx'_b, \quad (2.11)$$

where the term between braces is identified as the initial density matrix $\rho(x_a, x'_a, t_a)$ of the system, since

$$\rho(x, x', t) = \langle x | \rho | x' \rangle = \sum_{n} \langle x | n \rangle P(n, t) \langle n | x' \rangle.$$
(2.12)

Because of the orthonormality of the states, the probability to be in a state $|n_b\rangle$ at time t_b can also be extracted from the density matrix by

$$P(n_b, t_b) = \iint \langle x'_b | n_b \rangle \langle n_b | x_b \rangle \rho(x_b, x'_b, t_b) \, \mathrm{d}x_b \mathrm{d}x'_b.$$
(2.13)

It follows, by comparison with Eq.(2.11), that the density matrix at time t_b is given by

$$\rho(x_b, x'_b, t_b) = \iint K(x_b, t_b | x_a, t_a) K^*(x'_b, t_b | x'_a, t_a) \rho(x_a, x'_a, t_a) dx_a dx'_a.$$
(2.14)

Defining the propagator K_w of the Wigner function as

$$f(x_b, p_b, t_b) = \iint K_w(x_b, p_b, t_b | x_a, p_a, t_a) f(x_a, p_a, t_a) dx_a dp_a, \qquad (2.15)$$

one may extract it from Eq. (2.14) by using the Weyl transform (2.1) and its inverse:

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \iint \frac{\mathrm{d}\xi_b \mathrm{d}\xi_a}{2\pi\hbar} \exp\left(-\frac{i}{\hbar} \left(p_b \xi_b - p_a \xi_a\right)\right) \times K\left(x_b + \frac{\xi_b}{2}, t_b | x_a + \frac{\xi_a}{2}, t_a\right) K^*\left(x_b - \frac{\xi_b}{2}, t_b | x_a - \frac{\xi_a}{2}, t_a\right).$$
(2.16)

Introducing Feynman's path integral for the propagator K we arrive at

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \iint \int_{x(t_a) = x_a}^{x(t_b) = x_b} \int_{\xi(t_a) = \xi_a}^{\xi(t_b) = \xi_b} \mathcal{D}x \mathcal{D}\xi \exp\left(\frac{i}{\hbar}\Phi\left[x, p, \xi\right]\right) \frac{\mathrm{d}\xi_b \mathrm{d}\xi_a}{2\pi\hbar}, \quad (2.17)$$

where

$$\Phi\left[x, p, \xi\right] = -p\xi|_{t_a}^{t_b} + S\left[x + \frac{\xi}{2}\right] - S\left[x - \frac{\xi}{2}\right].$$

Note that the explicit time dependence in the path variables x(t) and $\xi(t)$ is omitted in order not to overload the notations. So far we have not really gained anything as compared to Feynman's path integral formulation for pure states. A significant simplification however arrises for systems that possess Galilean invariance. Consider x, for example, to be the coordinate of a particle with mass m in an external potential V(x), described by the action

$$S[x] = \int_{t_a}^{t_b} \left(\frac{m}{2}\dot{x}^2 - V(x)\right) dt.$$
 (2.18)

One then finds

$$S\left[x+\frac{\xi}{2}\right] - S\left[x-\frac{\xi}{2}\right] = \int_{t_a}^{t_b} \left[m\dot{x}\dot{\xi} - V\left(x+\frac{\xi}{2}\right) + V\left(x-\frac{\xi}{2}\right)\right] \mathrm{d}t$$

After an integration by parts for the kinetic term one obtains the following expression for the propagator K_w :

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \iint \int_{x(t_a)=x_a}^{x(t_b)=x_b} \int_{\xi(t_a)=\xi_a}^{\xi(t_b)=\xi_b} \mathcal{D}x \mathcal{D}\xi \exp\left(\frac{i}{\hbar} (m\dot{x} - p)\xi|_{t_a}^{t_b}\right) \times \\ \times \exp\left\{-\frac{i}{\hbar} \int_{t_a}^{t_b} \left[m\ddot{x}\xi + V\left(x + \frac{\xi}{2}\right) - V\left(x - \frac{\xi}{2}\right)\right] \mathrm{d}t\right\} \frac{\mathrm{d}\xi_b \mathrm{d}\xi_a}{2\pi\hbar}.$$

By definition the path integral over ξ sums over all possible paths between two fixed points (ξ_a, ξ_b) . Due to the Wigner-Weyl transformation one however has to integrate over all possible initial and final points (ξ_a, ξ_b) . Performing this last integral results in an unconstrained path integral over all possible paths. Moreover, the integral over the boundary term can be used to fix the initial and final momentum p to $m\dot{x}$, which confirms Wigner's statement that the p in expression (2.1) should be interpreted as the momentum conjugate to x. This finally brings us to

$$K_w\left(x_b, p_b, t_b | x_a, p_a, t_a\right) = \int_{\substack{p(t_b) = m\dot{x}_b \\ p(t_a) = m\dot{x}_a}}^{x(t_b) = x_b} \mathcal{D}x \int \frac{\mathcal{D}\xi}{2\pi\hbar} \exp\left\{-\frac{i}{\hbar} \int_{t_a}^{t_b} \left[m\ddot{x}\xi + V\left(x + \frac{\xi}{2}\right) - V\left(x - \frac{\xi}{2}\right)\right] \mathrm{d}t\right\}$$
(2.19)

The present formulation of the propagator, although completely equivalent to Feynman's formulation, is structurally different. Whereas both paths bear the same physical meaning in Feynman's double path integral formulation, the ξ path integral in expression (2.19) is completely auxiliary. The path integral over the physical variable x is now constrained by four boundary conditions rather than two. It is clear that, analogous to Feynman's path integral, the double path integral (2.19) can only be solved analytically for a limited set of problems. This new formulation, although mathematically equivalent to ordinary quantum theory, offers a distinct advantage for certain problems. Aside from this, the present formulations offers a new point of view, that might allow new insight. Before we enter this new terrain let us investigate some general properties and specific, well known, examples.

First note that it follows from the basic definition that the propagator is normalized

$$\forall \{x_a, p_a, t_a\}: \iint K_w(x, p, t | x_a, p_a, t_a) \,\mathrm{d}x \mathrm{d}p = 1$$
(2.20)

Although there is a complex weight for every path, the propagator is real. For every path $\xi(t)$ there is a path $-\xi(t)$ with exactly the opposite phase. Consequently the propagator can also be written as

$$K_w\left(x_b, p_b, t_b | x_a, p_a, t_a\right) = \int_{\substack{p(t_a) = m\dot{x}_a \\ p(t_a) = m\dot{x}_a}}^{x(t_b) = x_b} \mathcal{D}x \int \frac{\mathcal{D}\xi}{2\pi\hbar} \cos\left\{\int_{t_a}^{t_b} \left[m\ddot{x}\xi + V\left(x + \frac{\xi}{2}\right) - V\left(x - \frac{\xi}{2}\right)\right] \frac{\mathrm{d}t}{\hbar}\right\}.$$

$$(2.21)$$

It is clear that the propagator is thus real but not necessarily positive. Consequently the propagator K_w is a quasi conditional probability rather than a true conditional probability. It follows immediately from the basic definition in terms of wave function propagators that the Wigner propagator satisfies the Chapman-Kolmogorov equation or composition rule

$$K_{w}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a}) = \iint K_{w}(x_{b}, p_{b}, t_{b}|x, p, t) K_{w}(x, p, t|x_{a}, p_{a}, t_{a}) \,\mathrm{d}x\mathrm{d}p.$$
(2.22)

This property will be extensively used later. Note that, since we can use the composition rule in succession as many times as we want, it implies that the boundary condition $p_{a,b} = m\dot{x}_{a,b}$ must also be satisfied at all intermediate times t. An explicit path for the momentum variable can thus be constructed. The previous double path integral for the propagator can consequently also be written in terms of a quadruple path integral

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \int_{p(t_a)=p_a}^{p(t_b)=p_b} \mathcal{D}p \iint \frac{\mathcal{D}\xi \mathcal{D}\kappa}{(2\pi\hbar)^2} \exp\left\{-\frac{i}{\hbar} \int_{t_a}^{t_b} \left[\left(\frac{p}{m} - \dot{x}\right)\kappa + \dot{p}\xi + V\left(x + \frac{\xi}{2}\right) - V\left(x - \frac{\xi}{2}\right)\right] \mathrm{d}t\right\}.$$

The latter would have been obtained immediately from the definition if we would have used phase space path integral [18] rather than configuration space path integrals to define the initial wave function propagator. For completeness I would like to note that this representation is the key to generalize the propagator to actions which do not necessarily have Galilean invariance. Indeed, for any Lagrangian, even those that are not quadratic in velocity, we can use the phase space representation of the propagator

$$K(x_b, t_b | x_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \int \mathcal{D}p \exp\left\{\frac{i}{\hbar} \int_{t_a}^{t_b} \left[p\dot{x} - H(x, p)\right] dt\right\},$$
(2.23)

where the Hamiltonian H(x, p) is the Legendre transform of the original Lagrangian. Doing exactly the same exercise as for the configuration space path integral, we arrive at the following expression for the propagator

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \int_{p(t_a)=p_a}^{p(t_b)=p_b} \mathcal{D}p \iint \frac{\mathcal{D}\xi \mathcal{D}\kappa}{(2\pi\hbar)^2} \exp\left\{-\frac{i}{\hbar} \int_{t_a}^{t_b} \left[\dot{p}\xi - \dot{x}\kappa + H\left(x + \frac{\xi}{2}, p + \frac{\kappa}{2}\right) - H\left(x - \frac{\xi}{2}, p - \frac{\kappa}{2}\right)\right] \mathrm{d}t\right\}.$$
 (2.24)

As compared to (2.19) the phase is not just determined by the difference in potential $V(x+\xi/2)-V(x-\xi/2)$ but rather by the difference in the Hamiltonian $H\left(x+\frac{\xi}{2},p+\frac{\kappa}{2}\right)-H\left(x-\frac{\xi}{2},p-\frac{\kappa}{2}\right)$. Each of both auxiliary variables is furthermore multiplied by the time derivative of the conjugate variable. Note the difference in sign between the $\dot{p}\xi$ and $\dot{x}\kappa$ term, in agreement with (2.1), which is related to the underlying symplectic structure of phase space.

2.2.1 The Wigner-Liouville equation

The progagator for the Wigner distribution should of course also be the Green's function of the Wigner-Liouville equation. In order to see how this comes about, let us propagate a certain Wigner distribution over a time lapse $\epsilon \to 0$

$$f(x, p, t+\epsilon) = \iint K_w(x, p, t+\epsilon | x', p', t) \quad f(x', p', t) \, \mathrm{d}x' \mathrm{d}p'.$$
(2.25)

In this way expression (2.24) can be expanded for very short times

$$\lim_{\epsilon \to 0} K_w(x, p, t + \epsilon | x', p', t) = \iint \frac{\mathrm{d}\xi \mathrm{d}\kappa}{(2\pi\hbar)^2} \exp\left\{-\frac{i}{\hbar}\left[(p - p')\xi - (x - x')\kappa\right]\right\} \times \exp\left\{-\frac{i\epsilon}{\hbar}\left[H\left(x' + \frac{\xi}{2}, p' + \frac{\kappa}{2}, t\right) - H\left(x' - \frac{\xi}{2}, p' - \frac{\kappa}{2}, t\right)\right]\right\}.$$
 (2.26)

Since the time lapse is infinitesimal we can expand the second line up to first order in ϵ which yields the following expression for the distribution at time $t + \epsilon$

$$f(x, p, t+\epsilon) = f(x, p, t) - \frac{i\epsilon}{\hbar} \iiint \inf \left\{ -\frac{i}{\hbar} \left[(p-p')\xi - (x-x')\kappa \right] \right\} \times \left[H\left(x' + \frac{\xi}{2}, p' + \frac{\kappa}{2}, t\right) - H\left(x' - \frac{\xi}{2}, p' - \frac{\kappa}{2}, t\right) \right] f(x', p', t) \frac{\mathrm{d}\xi \mathrm{d}\kappa \mathrm{d}x'\mathrm{d}p'}{\left(2\pi\hbar\right)^2} + O(\epsilon^2). \quad (2.27)$$

Finally we identify

$$f(x, p, t + \epsilon) - f(x, p, t) \approx \frac{\partial f(x, p, t)}{\partial t}\epsilon,$$

from which we find the Wigner-Liouville equation for the distribution function

$$\frac{\partial f(x, p, t)}{\partial t} = -\frac{i}{\hbar} \iiint \exp\left\{-\frac{i}{\hbar} \left[(p - p')\xi - (x - x')\kappa\right]\right\} \times \left[H\left(x' + \frac{\xi}{2}, p' + \frac{\kappa}{2}, t\right) - H\left(x' - \frac{\xi}{2}, p' - \frac{\kappa}{2}, t\right)\right] f(x', p', t) \frac{\mathrm{d}\xi \mathrm{d}\kappa \mathrm{d}x'\mathrm{d}p'}{(2\pi\hbar)^2}.$$
 (2.28)

At this point let me just note that, by definition of the Moyal bracket [27] $\{\cdot, \cdot\}_M$, this can also be rewritten as

$$\frac{\partial f(x,p,t)}{\partial t} - \left\{ H(x,p,t), f(x,p,t) \right\}_M = 0.$$
(2.29)

In this way the Wigner-Liouville equation is reminiscent to the classical Liouville equation. In fact the Moyal bracket is a deformation of the Poisson bracket where Planck's constant controls the deformation such that for $\hbar \to 0$ the Moyal bracket tends to the Poisson bracket. Although this can be extracted from Eq. (2.28) it is more apparent in the operator representation of the Moyal bracket. Alternative to Eq. (2.28) and Eq. (2.29) one can define the Moyal bracket of two Wigner distributions f and g in terms of left and right derivatives as

$$\left\{f,g\right\}_{M} = f(x,p) \left[\frac{2}{\hbar}\sin\left(\frac{\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)\right)\right]g(x,p),$$

where $\overrightarrow{\partial}$ denotes the usual right derivative and $\overleftarrow{\partial}$ implies the derivative acts on the function to the left of the operator. Note that one can immediately define the Poisson bracket $\{\cdot, \cdot\}$ in a similar way as

$$\{f,g\} = f(x,p) \left(\frac{\overleftarrow{\partial}}{\partial x} \frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p} \frac{\overrightarrow{\partial}}{\partial x} \right) g(x,p).$$

Consequently the Moyal bracket can be defined in terms of the Poisson bracket as

$$\{\cdot,\cdot\}_M = \frac{2}{\hbar} \sin\left(\frac{\hbar}{2}\{\cdot,\cdot\}\right),$$

which for $\hbar \to 0$ results in the following statement

$$\{\cdot, \cdot\}_M = \{\cdot, \cdot\} + O(\hbar^2).$$
(2.30)

The implications will be discussed later. Elementary algebra furthermore allows to rewrite equation (2.28) as

$$i\hbar\frac{\partial f(x,p,t)}{\partial t} = H\left(x + \frac{i\hbar}{2}\frac{\partial}{\partial p}, p - \frac{i\hbar}{2}\frac{\partial}{\partial x}, t\right)f(x,p,t) - f\left(x + \frac{i\hbar}{2}\frac{\partial}{\partial p}, p - \frac{i\hbar}{2}\frac{\partial}{\partial x}, t\right)H(p,x,t)$$
(2.31)

At this point we recognize the Bopp representation (2.6) of the operators x and p at the right hand side of the equation. The inverse Weyl transformation of the last expression immediately yields the Von Neumann equation for the state of the system

$$i\hbar\frac{\partial\hat{\rho}}{\partial t} = \left[\hat{H}, \hat{\rho}\right]. \tag{2.32}$$

Note that this last step actually required H(x, p) to be the Weyl representation (2.4) of the Hamiltonian operator \hat{H} . This implies that the Hamiltonian in the phase space propagator (2.23) was also Weyl ordered, a point that is rarely mentioned. With hindsight this is logical since no ordering can ever be obtained from (2.23), so that the associated Hamiltonian operator should be completely symmetrically ordered and this is exactly what the Weyl ordering does. I just want to mention this fact for completeness and because it is relevant in chapter 4. At present this complication is rather academic since any physical Hamiltonian would automatically be symmetrically ordered.

2.2.2 Harmonic oscillator

Consider any time dependent harmonic potential

$$V(x,t) = a(t) + b(t)x + c(t)x^{2},$$

then

$$V\left(x+\frac{\xi}{2}\right) - V\left(x-\frac{\xi}{2}\right) = (b(t) + 2c(t)x)\xi.$$

In this case the propagator can be explicitly evaluated:

$$K_{w}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a}) = \int_{x(t_{a})=x_{a}}^{x(t_{b})=x_{b}} \mathcal{D}x \int_{p(t_{a})=p_{a}}^{p(t_{b})=p_{b}} \mathcal{D}p \int \int \frac{\mathcal{D}\xi \mathcal{D}\kappa}{(2\pi\hbar)^{2}}$$

$$\exp\left\{-\frac{i}{\hbar} \int_{t_{a}}^{t_{b}} \left[(\dot{p}+b(t)+2c(t)x)\xi - \left(\dot{x}-\frac{p}{m}\right)\kappa\right] dt\right\}$$

$$= \int_{x(t_{a})=x_{a}}^{x(t_{b})=x_{b}} \mathcal{D}x \int_{p(t_{a})=p_{a}}^{p(t_{b})=p_{b}} \mathcal{D}p\delta\left[\dot{p}+b\left(t\right)+2c\left(t\right)x\right]\delta\left[\dot{x}-\frac{p}{m}\right].$$
(2.33)

Out of all possible paths, only the classical phase space trajectory contributes to the path integral. This confirms the well known result [28] that the Wigner-Liouville equation can exactly be solved by the method of characteristics for all harmonic problems. The importance of the classical path for harmonic oscillators is also recognized in the usual Feynman path integral. For harmonic problems this propagator is indeed fully determined by the action of the classical trajectory. The link to classical mechanics is however even more clear in the present formulation since the quantum and classical dynamics are identical in this case.

I should stress that some care is required in interpreting this last result. A possible ambiguity arises because the path integral over the two delta *functionals* should result in two Dirac delta *functions* for the propagator. One could argue that it is a priori unclear what the argument of these Dirac delta functions should be. It follows immediately from properties (2.20) and (2.22) that the only natural way, natural in the sense that no additional normalization factor is required, is to solve both the equations of motion in a forward manner from the initial phase space point or backwards from the final phase space point, i.e.

$$K_{\text{quad}}(x_b, p_b, t_b | x_a, p_a, t_a) = \delta \left(x_b - x_{\text{cl}} \left(t_b | x_a, p_a, t_a \right) \right) \delta \left(p_b - p_{\text{cl}} \left(t_b | x_a, p_a, t_a \right) \right)$$
(2.34)

$$= \delta \left(x_a - x_{cl} \left(t_a | x_b, p_b, t_b \right) \right) \delta \left(p_a - p_{cl} \left(t_a | x_b, p_b, t_b \right) \right)$$
(2.35)

where $x_{cl}(t|x', p', t')$ and $p_{cl}(t|x', p', t')$ are the position and momentum at time t along the classical trajectory that passes trough a point x' with momentum p' at time t'. Any other combination will result in an additional normalization factor, as discussed in detail in appendix A.

Which one of the two expressions is the most useful depends on the problem at hand. The latter is obviously more useful if one wishes to propagate the initial distribution function forward in time. If one is only interested in the expectation value of certain operator, one can use the former equation to propagate the Weyl representation of the operator back in time. In that sense the choice between the two is similar to the choice between the Schrödinger and the Heisenberg picture.

Finally I would like to note that since the quantum and classical dynamics of the distribution function are the same the quantum mechanical properties of the harmonic oscillator are fully contained in the initial distribution. As a consequence of Heisenberg's uncertainty principle the initial distribution function can not be squeezed to an arbitrary small area in phase space. In fact one can show that it is impossible to squeeze the distribution into an area smaller than $2\pi\hbar$. Heisenberg's uncertainty principle is just one of the aspects of quantum mechanics and any effect of quantum interference is missing from the dynamics of the harmonic oscillator.

In order to investigate the effect of interference and superposition in the present language let us turn our attention to the experiment designed to contain all the mystery of quantum mechanics [29].

2.3 Double-slit experiment

Consider the standard double-slit experiment set up as depicted in Fig.(2.1). A particle source is present at some position \mathbf{r}_a , at some distance from an impenetrable wall in which two holes are punched at a distance d_h from each other. Suppose we have some detector at position \mathbf{r}_b behind the wall which allows us to detect the particles emitted by the source. In the standard double slit experiment the detector only detects whether or not a particle arrives at the position \mathbf{r}_b . Imagine that we can do the experiment many, many times under identical circumstances such that we can do full quantum state tomography and reconstruct the Wigner distribution behind the slit.

The problem thus becomes that of finding the Wigner distribution behind the wall given the initial source distribution $f_0(\mathbf{r}_a, \mathbf{p}_a)$. The relation between the two is obviously given by the propagator, described in the previous section as a sum over all possible paths that connect two points. In the present situations the two slits however pose geometrical constraints on the



Figure 2.1: The double slit experiment setup.

paths, since there is no way to reach \mathbf{r}_b without going to either one of the holes. The geometrical constraints alter the completeness relation [18] which affects the structure of the path integral. In the present situation the amplitude to reach \mathbf{r}_b from some point \mathbf{r}_a can be analyzed as a succession of events. First the particle would have to move to the wall, pass trough one of the two slits after which it can move to \mathbf{r}_b . Whenever two things happen in succession the amplitudes must be multiplied, such that the total propagator can be written as

$$K(\mathbf{r}_b, t_b | \mathbf{r}_a, t_a) = \int \mathrm{d}\mathbf{r} K_0(\mathbf{r}_b, t_b | \mathbf{r}, t) w(\mathbf{r}) K_0(\mathbf{r}, t | \mathbf{r}_a, t_a), \qquad (2.36)$$

where K_0 is the propagator without the geometrical constraint and $w(\mathbf{r})$ is a selection function that selects only those paths that pass trough a hole. By combining expression (2.36) and (2.16) the true Wigner propagator can be related to the Wigner propagator without geometrical constraints. Elementary algebra yields

$$K_{w}\left(\mathbf{r}_{b},\mathbf{p}_{b},t_{b}|\mathbf{r}_{a},\mathbf{p}_{a},t_{a}\right) = \iiint \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{p}'K_{0}\left(\mathbf{r}_{b},\mathbf{p}_{b},t_{b}|\mathbf{r},\mathbf{p},t\right)\Gamma\left(\mathbf{r},\mathbf{p}-\mathbf{p}'\right)K_{0}\left(\mathbf{r},\mathbf{p}',t|\mathbf{r}_{a},\mathbf{p}_{a},t_{a}\right),$$
(2.37)

where

$$\Gamma(\mathbf{r},\mathbf{p}) = \int w\left(\mathbf{r} + \frac{\boldsymbol{\xi}}{2}\right) w\left(\mathbf{r} - \frac{\boldsymbol{\xi}}{2}\right) \exp\left(-\frac{i}{\hbar}\mathbf{p} \cdot \boldsymbol{\xi}\right) \frac{\mathrm{d}\boldsymbol{\xi}}{2\pi\hbar}.$$
(2.38)

First of all note that $\Gamma(\mathbf{r}, \mathbf{p})$ is just the Wigner function corresponding to the selection function $w(\mathbf{r})$. Indeed, according to (2.1), a pure state $\hat{\rho} = |\psi\rangle \langle \psi|$, with $w(\mathbf{r}) = \langle \mathbf{r} |\psi\rangle$ would result in expression (2.38) for its Wigner distribution. Note that if the wall would not be there, $w(\mathbf{r}) = 1$ over the entire space, which implies $\Gamma(\mathbf{r}, \mathbf{p}) = \delta(\mathbf{p})$. By substituting this into expression (2.37) and using composition rule (2.22) one recovers the bare propagator. The true propagation of the distribution in time can be analyzed by a succession of three events. First the particles propagate for some time in the same way as they would without the presence of the wall to some position $(\mathbf{r}, \mathbf{p}')$. Next, the particle scatters in momentum space according to the slits' Wigner distribution $\Gamma(\mathbf{r}, \mathbf{p})$ after which it propagates again as if the wall would not be there. Furthermore note, just as in the classical case, that this allows us to find the Wigner function after the wall by propagating the distribution at the wall as if the wall is absent

$$f(\mathbf{r}_{b}, \mathbf{p}_{b}, t_{b}) = \iint \mathrm{d}\mathbf{r} \mathrm{d}\mathbf{p} K_{0}\left(\mathbf{r}_{b}, \mathbf{p}_{b}, t_{b} | \mathbf{r}, \mathbf{p}, t\right) f_{\mathrm{wall}}\left(\mathbf{r}, \mathbf{p}, t\right),$$

where we have defined the distribution function at the wall as

$$f_{\text{wall}}(\mathbf{r}, \mathbf{p}, t) = \iiint d\mathbf{p}' d\mathbf{r}_a d\mathbf{p}_a \Gamma(\mathbf{r}, \mathbf{p} - \mathbf{p}') K_0(\mathbf{r}, \mathbf{p}', t | \mathbf{r}_a, \mathbf{p}_a, t_a) f_0(\mathbf{r}_a, \mathbf{p}_a).$$



Figure 2.2: The slit Wigner function $\Gamma(y, p_y)$ for a single slit from y = -1 to y = 1. The corresponding marginal distributions are depicted at the back.

The crucial quantum mechanics is contained in the Wigner function $\Gamma(\mathbf{r}, \mathbf{p})$. The double slit selection function $w(\mathbf{r})$ can of course be expressed as $w(\mathbf{r}) = w_1(\mathbf{r}) + w_2(\mathbf{r})$, where w_1 and w_2 are the window functions of each of the holes separately. It is however immediately clear from expression (2.38) that the scattering function $\Gamma(\mathbf{r}, \mathbf{p}) \neq \Gamma_1(\mathbf{r}, \mathbf{p}) + \Gamma_2(\mathbf{r}, \mathbf{p})$, where Γ_1 and Γ_2 is the Wigner function of each of the holes separately. Instead we get

$$\Gamma(\mathbf{r},\mathbf{p}) = \Gamma_1(\mathbf{r},\mathbf{p}) + \Gamma_2(\mathbf{r},\mathbf{p}) + \int w_1\left(\mathbf{r} + \frac{\boldsymbol{\xi}}{2}\right) w_2\left(\mathbf{r} - \frac{\boldsymbol{\xi}}{2}\right) \cos\left(\mathbf{p} \cdot \boldsymbol{\xi}\right) \frac{\mathrm{d}\boldsymbol{\xi}}{\pi\hbar}$$

The two holes clearly interfere with each other, causing an interference pattern on a screen behind the two slits. The exact form of this pattern depends on the size and shape of the holes and on the shape of the initial distribution f_0 . Indeed, it is clear that even in the single slit experiment the result differs from the classical one where all particles either pass trough the slit undisturbed or reflect against the wall. The Wigner function $\Gamma(\mathbf{r}, \mathbf{p})$ for a single slit will contain oscillations if the slit has a finite width, as depicted in Fig.(2.2). Whereas the marginal real space distribution just depicts the shape of the slit, in agreement with the classical result, the marginal momentum distribution has oscillations determined by the slit width. A classical slit would however not change the momentum in any way. It is clear that the present analyses correctly predicts the (Fraunhofer) *diffraction* of the particles due to the slit. Moreover, in the ideal experiment, where the initial state is homogeneous in the direction parallel to the wall and does not travel in the direction parallel to the wall, the marginal momentum distribution of the slit's Wigner function is immediately related to the diffraction pattern on a screen far away from the slit.

The double slit Wigner function is depicted in Fig.(2.3). The figure indeed shows that the total Wigner distribution can not be analyzed as the sum of two single slit Wigner functions. The marginal position distribution however can. In contrast to the single slit distribution function the Wigner distribution is not necessarily zero whenever this marginal position distribution is zero. In between the two slits there is a region where the Wigner function oscillates strongly. It is exactly this part which is responsible for the interference and it is this part that can not be analyzed as the sum of two single slit Wigner distributions. In terms of the slit selection functions this part is the difference between a (classical) mixed state of two single slit functions and a *superposition* of two slits. Again the marginal momentum distribution is proportional



Figure 2.3: Wigner distribution $\Gamma(y, p_y)$ of a double slit experiment. The slits are separated by a distance which is 10 times larger than their width.

to the probability distribution on a screen far from the slits. It clearly shows an interference pattern with an envelope determined by the diffraction on each slit.

Finally I would like to remark that, although this is a standard setup to demonstrate the peculiarities of quantum mechanics, it is far from trivial to treat within the usual Hamiltonian Wigner function formalism. The difficulty arises from the fact that there is no consistent formulation [30] of the boundary value problem associated with the Wigner-Liouville equation (2.28). If one imposes Neumann boundary conditions to prevent any flow trough an impenetrable wall, just like one would to for a classical distribution function, one would just get the classical result back. From the basic definition of the Wigner function one can show that imposing Dirichlet boundary conditions on the wave function indeed results in Neumann boundary conditions on the distribution function but it results in Dirichlet boundary conditions at the same time, which implies there are to many conditions. The problem of imposing geometrical constraints on the Wigner-Liouville equation is in fact clearly illustrated by the double slit experiment itself. It is clear from Fig. (2.3) that there is a highly non local effect of the boundary condition which can not be obtained by simply imposing any boundary condition on the distribution in (2.28). One can argue that this problem can be avoided by making the geometrical constraints less stringent, i.e. by replacing the impenetrable wall with a finite potential, circumventing the need to impose additional boundary conditions. This however makes the propagator highly non harmonic and thereby analytically unsolvable.

2.4 Semiclassical approximations

The path integrals (2.19) and (2.24) appear to be only rarely analytically solvable. Similar to Feynman's path integrals, the fact that we can only do Gaussian integrals drastically restricts the number of solvable problems. The examples given in the previous section virtually exhaust the space of solvable problems. Almost any other analytically tractable problem somehow traces back to the harmonic oscillator or the double slit experiment.

In contrast, Barker and Murray conjecture in [16] that the time evolution of any Wigner

distribution is a linear superposition of classical time evolutions unfolded by a family of classical Hamiltonians according to a well defined prescription. This conjecture however immediately implies that only certain classical trajectories contribute to the path integral (2.24). It ought to be clear that this can not be true in general. In fact one can show that the conjecture is false [32] because the probability density is always equal to the classical probability density, which is only correct for the harmonic oscillator. A correct analysis in fact reveals that the time evolution of the Wigner distribution is a linear superposition of all possible evolutions with the weights given exactly by the path integral (2.24). Although the conjecture itself is false, it does recover the correct result for the harmonic oscillator. Let us therefore proceed by investigating different semi-classical approximations to the path integral, all of which will correctly recover the harmonic oscillator result but are different for non-harmonic problems.

2.4.1 Semiclassical truncated Wigner approximation

Wigner's original intention was to study quantum corrections to the classical thermodynamic potential, by expanding his distribution function in powers of \hbar . He concluded that, in thermal equilibrium, the first correction around the classical result is of order \hbar^2 . Such an expansion should thus also be possible for the dynamics of the system. In literature this expansion around the classical dynamics is known as the truncated Wigner approximation (TWA) [7]. In the Hamiltonian formulation it consists in truncating the Moyal bracket up to the classical Poisson bracket, hence the name. For harmonic problems we already know from the previous section that this truncation is exact. Note that \hbar does not appear anywhere anymore after the auxiliary path integral has been performed. This is the key to an expansion around the classical limit.

Recall that for a general Hamiltonian H(x, p) the propagator is given by expression (2.24). Let us now make the following substitution $\xi = \hbar \xi'$ and $\kappa = \hbar \kappa'$, and let me immediately drop the primes. Then the propagator becomes

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \int_{p(t_a)=p_a}^{p(t_b)=p_b} \mathcal{D}p \iint \frac{\mathcal{D}\xi \mathcal{D}\kappa}{(2\pi)^2} \exp\left\{-i \int_{t_a}^{t_b} \left[\dot{p}\xi - \dot{x}\kappa + \hbar^{-1}\left(H\left(x + \frac{\hbar\xi}{2}, p + \frac{\hbar\kappa}{2}\right) - H\left(x - \frac{\hbar\xi}{2}, p - \frac{\hbar\kappa}{2}\right)\right)\right] \mathrm{d}t\right\}.$$

At this point an \hbar -expansion of the Hamiltonian imposes itself

$$\hbar^{-1}\left(H\left(x+\frac{\hbar\xi}{2},p+\frac{\hbar\kappa}{2}\right)-H\left(x-\frac{\hbar\xi}{2},p-\frac{\hbar\kappa}{2}\right)\right)=\frac{\partial H}{\partial x}\xi+\frac{\partial H}{\partial p}\kappa+O\left(\hbar^{2}\right)$$

Note that the right hand side of the previous expression is linear in the auxiliary variables ξ and κ such that the path integrals over these variables can be done if we completely neglect all terms of order \hbar ² or higher, i.e., we find

$$K_{\text{TWA}}\left(x_{b}, p_{b}, t_{b} | x_{a}, p_{a}, t_{a}\right) = \int_{x(t_{a})=x_{a}}^{x(t_{b})=x_{b}} \mathcal{D}x \int_{p(t_{a})=p_{a}}^{p(t_{b})=p_{b}} \mathcal{D}p\delta\left[\dot{x} - \frac{\partial H}{\partial p}\right]\delta\left[\dot{p} + \frac{\partial H}{\partial x}\right]$$

Consequently only those trajectories that obey Hamilton's equations of motion contribute to the propagator. The semiclassical truncated Wigner approximation thus constitutes in classically propagating the initial state. Analogous to the harmonic oscillator, quantum effects are thereby only incorporated in the initial state. Corrections around this result are of order \hbar^2 and it thus appears adequate to set up a perturbation theory around the TWA. Let us therefore define the quantum correction

$$\Delta H_q(x,p;\xi,\kappa) = \hbar^{-1} \left(H\left(x + \frac{\hbar\xi}{2}, p + \frac{\hbar\kappa}{2}\right) - H\left(x - \frac{\hbar\xi}{2}, p - \frac{\hbar\kappa}{2}\right) \right) - \frac{\partial H}{\partial x}\xi + \frac{\partial H}{\partial p}\kappa, \quad (2.39)$$

as the difference between the full expression and the zeroth order term in its expansion. Then our propagator can be rewritten as

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \int_{p(t_a)=p_a}^{p(t_b)=p_b} \mathcal{D}p \iint \frac{\mathcal{D}\xi \mathcal{D}\kappa}{(2\pi)^2} \exp\left\{-i \int_{t_a}^{t_b} \left[\left(\dot{p} + \frac{\partial H}{\partial x}\right) \xi - \left(\dot{x} - \frac{\partial H}{\partial p}\right) \kappa + \Delta H_q(x, p; \xi, \kappa) \right] \mathrm{d}t \right\}.$$

Because ΔH_q is of order \hbar^2 we proceed by expanding the exponential in a series around $\Delta H_q = 0$. The contribution of order n to the propagator will be denoted K_n , such that for example $K_0 = K_{\text{TWA}}$. The first order correction around the TWA thereby becomes

$$K_{1}(x_{b}, p_{b}, t_{b} | x_{a}, p_{a}, t_{a}) = -i \int_{t_{a}}^{t_{b}} \mathrm{d}\tau \int_{x(t_{a})=x_{a}}^{x(t_{b})=x_{b}} \mathcal{D}x \int_{p(t_{a})=p_{a}}^{p(t_{b})=p_{b}} \mathcal{D}p \iint \frac{\mathcal{D}\xi \mathcal{D}\kappa}{(2\pi)^{2}} \Delta H_{q}(x, p; \xi, \kappa) \\ \exp\left\{-i \int_{t_{a}}^{t_{b}} \left[\left(\dot{p} + \frac{\partial H}{\partial x}\right)\xi - \left(\dot{x} - \frac{\partial H}{\partial p}\right)\kappa\right] \mathrm{d}t\right\}.$$

Introducing the Fourier representation of ΔH_q

$$\Delta H_q(x, p; \xi, \kappa) = i \iint dp' dx' \exp(ip'\xi - ix'\kappa) \Gamma(x, p; p', x'),$$

allows us to rewrite the first order correction as

$$K_{1}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a}) = \int_{t_{a}}^{t_{b}} \mathrm{d}\tau \iint \mathrm{d}p' \mathrm{d}x' \int_{x(t_{a})=x_{a}}^{x(t_{b})=x_{b}} \mathcal{D}x \int_{p(t_{a})=p_{a}}^{p(t_{b})=p_{b}} \mathcal{D}p\Gamma(x, p; p', x')$$
$$\iint \frac{\mathcal{D}\xi \mathcal{D}\kappa}{(2\pi)^{2}} \exp\left\{-i \int_{t_{a}}^{t_{b}} \left[\left(\dot{p} + \frac{\partial H}{\partial x} - p'\delta(t-\tau)\right)\xi - \left(\dot{x} - \frac{\partial H}{\partial p} - x'\delta(t-\tau)\right)\kappa\right] \mathrm{d}t\right\}.$$

This allows us to perform the auxiliary path integrals, after which we find

$$K_{1}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a}) = \int_{t_{a}}^{t_{b}} \mathrm{d}\tau \iint \mathrm{d}p' \mathrm{d}x' \int_{x(t_{a})=x_{a}}^{x(t_{b})=x_{b}} \mathcal{D}x \int_{p(t_{a})=p_{a}}^{p(t_{b})=p_{b}} \mathcal{D}p\Gamma(x, p; p', x')$$
$$\delta\left[\dot{p} + \frac{\partial H}{\partial x} - p'\delta(t-\tau)\right] \delta\left[\dot{x} - \frac{\partial H}{\partial p} - x'\delta(t-\tau)\right].$$

Although the result can immediately be interpreted from this expression, I prefer to rewrite it by using the composition rule (2.22). In this way we eliminate all path integrals and end up with

$$K_{1}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a}) = \int_{t_{a}}^{t_{b}} d\tau \iint dp dx \iint dp' dx' K_{0}(x_{b}, p_{b}, t_{b}|x', p', \tau) \Gamma(x, p; p' - p, x' - x) K_{0}(x, p, \tau|x_{a}, p_{a}, t_{a}).$$
(2.40)

Either way the first order correction to the semiclassical propagator is a semiclassical propagator with a single quantum jump. The quantum jump will scatter the particle from some momentum p and position x to a momentum p' and position x' with a quasi probability $\Gamma(x, p; p' - p; x' - x)$. In order to obtain the total first order correction we have to add all possible quantum jumps, i.e. of all possible size and at all possible times. The exact same



Figure 2.4: Diagrammatic representation of the perturbation series.



Figure 2.5: Dyson series for the propagator

procedure can be repeated for any remaining order in the perturbation series and it is clear that the n^{th} order will contain n quantum jumps, every jump adding at least a factor \hbar^2 to the propagator. Such processes can be depicted in a pictorial way in terms of Feynman-like diagrams in phase space, as depicted in Fig. (2.4). Note however that the diagrams do not have to be closed and all diagrams have the same (trivial) topology. An exact resummation of the series can therefore be performed by time ordering all the events. In this way we find the following integral equation for the propagator

$$K_{w}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a}) = K_{0}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a})$$

+
$$\int_{t_{a}}^{t_{b}} d\tau \iint dp dx \iint dp' dx' K_{0}(x_{b}, p_{b}, t_{b}|x', p', \tau) \Gamma(x, p; p' - p, x' - x) K_{w}(x, p, \tau | x_{a}, p_{a}, t_{a}).$$
(2.41)

It is clear that continuous resubstitution of the right hand side into the K_w in the second line will generate the complete perturbation series as illustrated in Fig. (2.5). Several interpretations and practical implementations of this perturbation around the semiclassical propagator exist besides the one presented here. First of all, one finds that the scattering function $\Gamma(x, p; p', x')$



Figure 2.6: Perturbation expansion in terms of particle–antiparticle generation events.

is and odd function of p' and x' such that

$$\iint \mathrm{d}p' \mathrm{d}x' \Gamma\left(x, p; p', x'\right) = 0$$

This implies particle number conservation. Indeed since the semiclassical propagator conserves the particle number, all higher order propagators should have an average quasi density of zero. Instead of the interpretation of the series in terms of scattering diagrams one can thus think of every event in terms of the generation of a *particle-antiparticle* pair as shown in Fig. (2.6). Here particles should just be interpreted as Monte Carlo samples of the distribution. The expansion in this way becomes an expansion in the number of particle-antiparticle pair production events around the semiclassical propagator. This interpretation clearly shows the exponential complexity of quantum mechanics. The number of particles now increases exponentially with the order in the perturbation series. Note that this is just a different interpretation of the diagrams but it is still the same perturbation series. The exponential complexity in the first diagrammatic representation also resides in the fact that the quasi probability for a jump is an odd function of the p' and x'. In half of the scattering events the propagator will thus change sign. A sign problem presents itself and the complexity consequently scales exponentially in the order of the series as it becomes increasingly more difficult to get any statistically relevant result. The order in the perturbation theory is in fact similar to the number of fermions in the fermionic sign problem.

Another scheme can be given to implement quantum corrections. In the previous discussion we just subtracted the classical part from the total action and expanded everything in the quantum correction. This quantum correction (2.39) itself is actually built up out of different orders in \hbar^2 . A full expansion of (2.39) yields

$$\Delta H_q(x,p;\xi,\kappa) = \sum_{n,m=0}^{\infty} \frac{1}{n!m!} \left(\frac{\hbar}{2}\right)^{n+m-1} \frac{\partial^{n+m}H}{\partial x^n \partial p^m} \xi^n \kappa^m , \qquad (2.42)$$

where $n + m \neq 1$ and n + m should be odd, as all even terms drop out because of symmetry. Consequently Γ can be written as

$$\Gamma\left(x,p;p',x'\right) = \sum_{n,m=0}^{\infty} \frac{\left(-1\right)^{m+1}}{n!m!} \left(\frac{\hbar}{2}\right)^{n+m-1} \frac{\partial^{n+m}H}{\partial x^n \partial p^m} \delta^{(n)}(p') \delta^{(m)}(x') , \qquad (2.43)$$



Figure 2.7: Moyal expansion of the pertrubation series.

where the same conditions hold for n and m, and where $\delta^{(i)}(x)$ denotes the i^{th} derivative of a Dirac delta function. Since n+m should be odd we have n+m-1=2l, such that all terms with the same l have an overall prefactor \hbar^{2l} . We can therefore define

$$\Gamma(x,p;p',x') \equiv \sum_{l=1}^{\infty} \Gamma_l(x,p;p',x') ,$$

where the restriction $n + m \neq 1$ implies $l \geq 1$. Instead of doing the perturbation series in the number of scattering events or pair productions N we can now organize the series in terms of \hbar^2 , consequently in fixed lN. This approach, although completely equivalent if done up to all orders is fundamentally different from the other two when it is truncated at some finite order m = lN. Note that the exponential complexity has not been mysteriously removed. On the contrary it has even been increased. It is clear from Fig. (2.7) that every m = lN order contains one diagram that is fully equivalent to the diagrams in Fig. (2.4), i.e. the diagram with l = 1 and m = N. Hence the number of pairs still increases exponentially. From expression (2.43) we also see that the other diagrams with higher l but lower number of scatterings will have more nodes in the scattering function itself. In fact two more nodes appear every time l is increased by one. In order to efficiently capture this nodal structure one has to increase the sampling in the same way as in the original perturbation series. In this expansion an additional complication arises in the sense that the number of topologically different diagrams also increases factorial in lN.

Even though we have now expanded everything in orders of \hbar^2 it is hard to imagine that any convergent result can be obtained from (2.43) since it becomes increasingly more singular when we increase the order. Indeed the perturbation Γ can hardly be considered to be small as compared to the propagator and the series can strictly speaking never converge. However the final effect of a perturbation can be weak for certain initial states. An integration by parts in expression (2.40) with Γ given by (2.43) allows to shift the derivatives from the scattering term to the propagator such that if we apply it on a certain initial distribution we get derivatives of the distribution function. Note that this is exactly the Moyal expansion of the Wigner kernel in the Hamiltonian formulation. Consequently the effect of the quantum jumps becomes weak whenever the change of the distribution function is weak compared to the change of the Hamiltonian with the conjugate variable, because the overall weight of the n, m correction scales like

$$\frac{\partial^{n+m}H}{\partial x^n \partial p^m} \frac{\partial^{n+m}f}{\partial p^n \partial x^m}.$$

If we apply this to the double-slit experiment described in the previous section, where the momentum part is simply quadratic but the potential changes abruptly, we see that in order for the corrections to be small and thus for the perturbation theory to be sensible, the distribution function must be spread over momentum space. This is exactly the opposite limit of the ideal experiment described before. In this limit the interference pattern disappears because the convolution of this broad initial distribution with the slit Wigner function depicted in Fig.(2.3) will wash out all the oscillations in the superposition part between the two slits. This clearly shows that sensible results can be obtained by expanding around the classical trajectory if the final result is more or less classical. It is important to note that whether or not this is the case does not just depend on the Hamiltonian of the system but is intrinsically linked to the initial state as indicated by the previous example.

2.4.2 Variational truncated Wigner approximation

In this section we present a method to extract the effective classical Hamiltonian associated with the optimal classical phase space evolution. The overall goodness of the previous expansion around the classical trajectory is unclear. Although each quantum jump carries an additional \hbar^2 both schemes neccessarilly have a component which makes every propagator more singular than the propagator of the previous order. We however realized that the effect of the quantum jumps on the state, rather than on the propagator, can be extremely weak depending on the shape of the initial state as compared to the behavior of the Hamiltonian. Consequently the goodness of the expansion ought to be determined by comparing states rather than propagators. In order to assess the goodness of the result we thus have to define a metric on Hilbert space. Many different distance measures have been defined in the context of quantum information theory. Here we adopt the Hilbert-Schmidt norm to define the distance, i.e.

$$\left\|\hat{\rho}\right\|_{2} = \sqrt{\operatorname{Tr}\left[\hat{\rho}^{\dagger}\hat{\rho}\right]}.$$

Although it lacks the operation interpretation [31] of the trace norm $\|\cdot\|_1$, it is mathematically more friendly in use and can directly be expressed in phase space. Moreover note that the squared Hilbert-Schmidt norm is equal to the purity of the state. If we denote the Wigner function associated with state $\hat{\rho}$ and $\hat{\sigma}$ as $f_{\rho}(x, p)$ and $f_{\sigma}(x, p)$ respectively, then the Hilbert-Schmidt distance between the two states is given by

$$D_2(\hat{\rho},\hat{\sigma}) = \sqrt{\mathrm{Tr}\left[\left(\hat{\rho}-\hat{\sigma}\right)^{\dagger}\left(\hat{\rho}-\hat{\sigma}\right)\right]} = \sqrt{2\pi\hbar} \iint \mathrm{d}x \mathrm{d}p \left(f_{\rho}(x,p,t)-f_{\sigma}(x,p,t)\right)^2.$$
(2.44)

Next consider f_{ρ} to be the true Wigner function, generated from an initial state f_0 by propagating it with the true propagator (2.24). On the other hand f_{σ} is an approximation to f_{ρ} generated from the same initial state f_0 by propagating it with a semiclassical approximation. Instead of simply approximating the time evolution of the system by its classical time evolution, let us allow the classical Hamiltonian to differ from the original one. I.e., we take

$$K_{\sigma}\left(x_{b}, p_{b}, t_{b} | x_{a}, p_{a}, t_{a}\right) = \int_{x(t_{a})=x_{a}}^{x(t_{b})=x_{b}} \mathcal{D}x \int_{p(t_{a})=p_{a}}^{p(t_{b})=p_{b}} \mathcal{D}p\delta\left[\dot{x} - \frac{\partial H_{\sigma}}{\partial p}\right]\delta\left[\dot{p} + \frac{\partial H_{\sigma}}{\partial x}\right], \quad (2.45)$$

where H_{σ} has yet to be determined. The optimal effective classical Hamiltonian H_{eff} is subsequently defined as the Hamiltonian H_{σ} that minimizes the Hilbert-Schmidt distance between the approximate and the true Wigner function

$$\frac{\delta D_2(\hat{\rho},\hat{\sigma})}{\delta H_\sigma}\Big|_{H_\sigma=H_{\text{eff}}} = 0.$$

Before we proceed and calculate the functional derivative, it is important to note that we suppose that one can not evaluate (2.24) exactly because we do not know the true Wigner

function. If this was known, we can of course calculate the effective classical Hamiltonian but this would be a rather academic exercise since we already have the exact answer. If we do not have the exact solution we must therefore somehow estimate the true Wigner function in order to find an estimate of the distance. If we were to have the optimal semiclassical approximation, our best guess of the true solution would be obtained by doing perturbation theory around this optimal classical state. In fact we can define the true propagator in terms of a Dyson series, analogous to (2.41), around the semiclassical guess K_{σ} . If we would be able to solve the complete Dyson series it is clear we have the exact solution and it does not depend on the effective classical Hamiltonian. However, we will necessarily have to truncate the series up to a finite order which will make our guess of the exact solution depend on the effective classical Hamiltonian itself. In other words, although the true distance depends only on H_{σ} trough the trial state $\hat{\sigma}$, the optimal estimation of this distance also depends on H_{σ} trough the optimal estimation of the exact solution. There is thus a clear distinction between minimizing the distance under the assumption that f_{ρ} is known exactly or with the knowledge that f_{ρ} depends on H_{σ} .

In order to minimize the distance with respect to the effective classical Hamiltonian we introduce the propagator in expression (2.44) which results in

$$\frac{D_2^2(\hat{\rho},\hat{\sigma})}{2\pi\hbar} = \iint \mathrm{d}x_b \mathrm{d}p_b \left(\iint \mathrm{d}x_a \mathrm{d}p_a \left[K_w\left(x_b, p_b, t_b | x_a, p_a, t_a\right) - K_\sigma\left(x_b, p_b, t_b | x_a, p_a, t_a\right)\right] f_0(x_a, p_a)\right)^2$$

next we expand the exact propagator in a perturbation series around K_{σ} . At present we will restrict the discussion to first order perturbation theory

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) \approx K_\sigma(x_b, p_b, t_b | x_a, p_a, t_a)$$

+
$$\int_{t_a}^{t_b} d\tau \iint dp dx \iint dp' dx' K_\sigma(x_b, p_b, t_b | x', p', \tau) \Gamma_\sigma(x, p; p' - p, x' - x) K_\sigma(x, p, \tau | x_a, p_a, t_a).$$

Here the scattering amplitude Γ is given by

$$\Gamma_{\sigma}(x,p;p',x') = -\frac{i}{\hbar} \iint \exp\left(-\frac{i}{\hbar}\left(p'\xi - x'\kappa\right)\right) \Delta H_{\sigma}(x,p;\xi,\kappa) \frac{\mathrm{d}\kappa \mathrm{d}\xi}{\left(2\pi\hbar\right)^2},\tag{2.46}$$

with

$$\Delta H_{\sigma}\left(x,\xi;p,\kappa\right) = \left(H\left(x+\frac{\xi}{2},p+\frac{\kappa}{2}\right) - H\left(x-\frac{\xi}{2},p-\frac{\kappa}{2}\right)\right) - \frac{\partial H_{\sigma}}{\partial x}\xi + \frac{\partial H_{\sigma}}{\partial p}\kappa.$$
 (2.47)

Note that this is completely analogous to the scattering amplitude in the previous section. We have just subtracted the effective classical Hamiltonian from the full action rather than the real Hamiltonian. In this way the (squared) Hilbert-Schmidt distance becomes

$$\frac{D_2^2(\hat{\rho},\hat{\sigma})}{2\pi\hbar} = \iint \mathrm{d}x_b \mathrm{d}p_b \left(\iint \mathrm{d}x_a \mathrm{d}p_a \int_{t_a}^{t_b} \mathrm{d}\tau \iint \mathrm{d}p \mathrm{d}x \iint \mathrm{d}p' \mathrm{d}x' K_\sigma \left(x_b, p_b, t_b | x', p', \tau \right) \times \Gamma_\sigma \left(x, p; p' - p, x' - x \right) K_\sigma \left(x, p, \tau | x_a, p_a, t_a \right) f_0(x_a, p_a) \right)^2.$$

Although this expression looks rather horrible it can easily be represented as a diagram, as depicted in Fig. (2.8). The diagram can be read in two different ways. Either one thinks of it as two copies of the state propagating in time until time t_b after which we take the product of the two and integrate over space. Or the diagram is interpreted as a single state evolving to time t_b after which it evolves backwards in time to the initial state t_a at which point we



Figure 2.8: First order approximation of the Hilbert-Schmidt distance.

multiply it with the initial state and integrate it out. The latter interpretation is reminiscent of the Schwinger-Keldysh contour. The final point (x_b, p_b) can be integrated out by using the composition rule (2.22) because it simply connects two propagators. Note that this is allowed because of time reversal symmetry of the underlying problem. This yields the following expression for the Hilbert-Schmidt distance

$$\frac{D_2^2(\hat{\rho},\hat{\sigma})}{2\pi\hbar} = \int_{t_a}^{t_b} \mathrm{d}\tau_2 \int_{t_a}^{t_b} \mathrm{d}\tau_1 \iint \mathrm{d}p_2 \mathrm{d}x_2 \iint \mathrm{d}p'_2 \mathrm{d}x'_2 \iint \mathrm{d}p_1 \mathrm{d}x_1 \iint \mathrm{d}p'_1 \mathrm{d}x'_1
f_{\sigma}\left(x_2, p_2, \tau_2\right) \Gamma_{\sigma}\left(x_2, p_2; p'_2 - p_2, x'_2 - x_2\right) \times
\times K_{\sigma}\left(x'_2, p'_2, \tau_2 | x'_1, p'_1, \tau_1\right) \Gamma_{\sigma}\left(x_1, p_1; p'_1 - p_1, x'_1 - x_1\right) f_{\sigma}\left(x_1, p_1, \tau_1\right). \quad (2.48)$$

It is clear that the effective Hamiltonian, if it were even possible to extract it from the previous expression, would depend non-locally on the distribution in time. Consider, for example, some Hamiltonian which minimizes the distance at time $t = t_b$. If we were to deform the contour to $t = t_b + \epsilon$, then the optimal Hamiltonian at this time could be different from the previous one over the entire interval (t_a, t_b) . This, in my opinion, beautifully illustrates the profound difference between Lagrangian and Hamiltonian dynamics. In the present situation it is however rather annoying because we would like to extract the Hamiltonian from this Lagrangian quantity which depends on the whole phase-space-time trajectory. It however shows that we would actually like to have the following situation instead. If we change the time by an infinitesimal part from $t = t_b$ to $t = t_b + \epsilon$, then we only which to determine the Hamiltonian in this small time interval while leaving the time evolution for all times $t \leq t_b$ intact.

Therefore we only need to study the distance over a very small time increment $t_b = t + \epsilon$ and $t_a = t$, with $\epsilon \to 0$, such that we find

$$\frac{\Delta D_2^2(\rho,\sigma)}{2\pi\hbar} = \epsilon^2 \iint dp_2 dx_2 \iint dp'_2 dx'_2 \iint dp_1 dx_1 \iint dp'_1 dx'_1 f_{\sigma}(x_2, p_2, t) \Gamma_{\sigma}(x_2, p_2; p'_2 - p_2, x'_2 - x_2) K_{\sigma}(x'_2, p'_2, t | x'_1, p'_1, t) \Gamma_{\sigma}(x_1, p_1; p'_1 - p_1, x'_1 - x_1) f_{\sigma}(x_1, p_1, t).$$

By construction of the propagator it becomes a delta function when both the time arguments are equal. Integrating out this delta function yields

$$\frac{\Delta D_2^2(\hat{\rho},\hat{\sigma})}{2\pi\hbar} = \epsilon^2 \iint \mathrm{d}x' \mathrm{d}p' \left[\iint \mathrm{d}x \mathrm{d}p \Gamma_\sigma\left(x,p;p'-p,x'-x\right) f_\sigma(x,p,t) \right]^2.$$

The expression is now free of any propagators. It depends on the present distribution only. This distribution of course depends on all previous effective Hamiltonians but that is the past and we do not wish to alter it. If we furthermore combine the expressions (2.46) and (2.47), and compare the result with expressions (2.28) and (2.29) we find

$$\frac{\Delta D_2^2(\hat{\rho},\hat{\sigma})}{2\pi\hbar} = \epsilon^2 \iint \mathrm{d}x \mathrm{d}p \left(\{H(x,p,t), f_\sigma(x,p,t)\}_M - \{H_\sigma(x,p,t), f_\sigma(x,p,t)\} \right)^2.$$
(2.49)

This expression can finally be minimized with respect to H_{σ} which results in the following Euler-Lagrange equation for the effective classical Hamiltonian

$$\{\{H_{\text{eff}}(x, p, t), f_{\sigma}(x, p, t)\}, f_{\sigma}(x, p, t)\} = \{\{H(x, p, t), f_{\sigma}(x, p, t)\}_{M}, f_{\sigma}(x, p, t)\}.$$
 (2.50)

This is the main result of this section. It tells us how to find the effective classical Hamiltonian given the present trial state and the present Hamiltonian. Although the trial state itself can depend on all the previous H_{eff} , they only influence the present effective Hamiltonian trough the Wigner distribution at the present time. Moreover, note that since the trial state is propagated classically according to (2.45) it satisfies following equation of motion

$$\frac{\partial f_{\sigma}(x,p,t)}{\partial t} - \{H_{\sigma}(x,p,t), f_{\sigma}(x,p,t)\} = 0.$$

One can substitute this into the expression for the effective Hamiltonian which then reads

$$\left\{\frac{\partial f_{\sigma}(x,p,t)}{\partial t} - \left\{H(x,p,t), f_{\sigma}(x,p,t)\right\}_{M}, f_{\sigma}(x,p,t)\right\} = 0.$$
(2.51)

Recall that the exact distribution satisfies (2.29), such that the first argument in the Poisson bracket vanishes whenever the trial distribution satisfies the exact Liouville equation. This is of course a particular way to make the Poisson bracket vanish, it is however not guaranteed that this limit can be obtained. In general the trial equation of motion is thus equal to the real equation of motion up to a jump distribution or an effective Boltzmann collision term which is in mutual involution with the trial distribution, i.e.

$$\frac{\partial f_{\sigma}}{\partial t} - \{H, f_{\sigma}\}_{M} = \left(\frac{\partial f_{\sigma}}{\partial t}\right)_{\text{jump}}$$
(2.52)

with
$$\left(\frac{\partial f_{\sigma}}{\partial t}\right)_{\text{jump}} = \{H_{\text{eff}}, f_{\sigma}\} - \{H, f_{\sigma}\}_{M}.$$
 (2.53)

If $\{(\partial_t f_\sigma)_{\text{jump}}, f_\sigma\} = 0$ and if H_{eff} is a solution of Eq. (2.50), the optimal trial distribution f_σ evolves classically. Whether or not this curious condition, that the effective jump distribution and the optimal classical trial distribution have vanishing Poisson brackets, can be used for anything useful is still under investigation.

Equation (2.50) is a linear inhomogeneous second-order partial differential equation with non-constant coefficients. It is clear that it can not be solved analytically in general. A possible way to simplify the problem is to parametrize the model Hamiltonian in order to include specific additional physics. In this way the minimization of the distance (2.49) will not result in a differential equation for the Hamiltonian but it will give a set of algebraic equations for the undetermined parameters in the model Hamiltonian. In [33] we contributed to this possibility in the context of quantum transport. In that work we minimized the distance under the ansatz that the effective Hamiltonian

$$H_{\text{eff}}(x,p) = \frac{p^2}{2m} + V_{\text{eff}}(x),$$

is parametrized by a scalar potential $V_{\text{eff}}(x)$. In this way we constructed a stable forward numerical integration scheme for the exact Wigner distribution. Although the optimization is strictly speaking not necessary in that case, one finds that the highly singular terms in the Wigner kernel (2.43) cause numerical instabilities which are largely removed by the optimization of the algorithm. Although extremely interesting an sich we will not explore this option here, since it does not improve in any way our understanding of the presented method.

Another option is to look for a solution of Eq. (2.50) for specific simple Wigner functions. Let me illustrate this approach here for the quartic oscillator. Although of limited practical interest, this example provides the required background for treating the contact potential in quantum field theory which is the content of the last chapter. The example is moreover instructive because it requires minimal mathematical effort to get the result and shows the desired effect. A general method to obtain the effective Hamiltonian for an arbitrary Gaussian Wigner function is presented in appendix B.

Gaussian initial state for a quartic oscillator

As an example, consider a one dimensional quartic oscillator

$$H = \frac{p^2}{2} + \frac{x^2}{2} + \frac{gx^4}{4},$$
(2.54)

expressed in natural units of the harmonic oscillator, i.e., $\hbar = m = \omega = 1$. In this case the Moyal expansion has a finite number of terms and becomes

$$\{H, f\}_M = \{H, f\} - \frac{gx}{4} \frac{\partial^3 f}{\partial p^3},$$
 (2.55)

with
$$\{H, f\} = (x + gx^3) \frac{\partial f}{\partial p} - p \frac{\partial f}{\partial x},$$
 (2.56)

Since the Moyal bracket is expanded in the Poisson bracket plus a correction, it is natural to expand the trial Hamiltonian as

$$H_{\rm eff} = H + H_c, \tag{2.57}$$

in which H_c accounts for the correction and satisfies the following partial differential equation

$$\{\{H_c, f_\sigma\}, f_\sigma\} = -\frac{g}{4} \left\{ x \frac{\partial^3 f_\sigma}{\partial p^3}, f_\sigma \right\}.$$
 (2.58)

As in any problem of quantum dynamics, the initial state has to be given, and can by no means be calculated. Because of the Heisenberg uncertainty principle, a reasonable example of an initial distribution function is a Gaussian wave packet in position and momentum. Although many other trial time evolutions can be imagined, we here illustrate the optimization method for a displaced version in time of this initial wave packet:

$$f_{\sigma}(x, p, t) = \frac{1}{2\pi\sigma_x\sigma_p} \exp\left(-\frac{(x - x_0(t))^2}{2\sigma_x^2} - \frac{(p - p_0(t))^2}{2\sigma_p^2}\right) \quad \text{with } 2\sigma_x\sigma_p \ge 1.$$
(2.59)

The condition $2\sigma_x \sigma_p \geq 1$ accounts for the uncertainty relation. With this trial distribution function, equation (2.58) can be solved since all derivatives of f, due to the Poisson brackets, result in Hermite polynomials such that the overall f_{σ}^2 factor drops out. The remaining second order equation consequently only contains polynomials. Its solution can thus be obtained in a simple way by the Frobenius method. Substituting the power series ansatz yields an algebraic set of equations from which we finally arrive at the following expression for the correction

$$H_{c} = \frac{x^{2}g}{48\sigma_{p}^{2}} \left(18 - x\frac{3x - 4x_{0}}{\sigma_{x}^{2}} - 6\frac{(p - p_{0})^{2}}{\sigma_{p}^{2}} \right) + u \left(\frac{(x - x_{0})^{2}}{2\sigma_{x}^{2}} + \frac{(p - p_{0})^{2}}{2\sigma_{p}^{2}} \right)$$

where u is an arbitrary function. The optimal effective Hamiltonian (2.57) along these lines thus becomes

$$H_{\text{eff}} = \frac{p^2}{2} + \left(1 + \frac{3g}{4\sigma_p^2}\right)\frac{x^2}{2} + \left(1 - \frac{1}{\left(2\sigma_x\sigma_p\right)^2}\right)\frac{gx^4}{4} + \frac{g}{\left(2\sigma_x\sigma_p\right)^2}\frac{x_0x^3}{3} - \frac{g}{4\sigma_p^4}\frac{x^2\left(p - p_0\right)^2}{2}.$$
 (2.60)

From this effective Hamiltonian one can calculate the effective jump distribution (2.53), which turns out to vanish, i.e., $(\partial_t f_{\sigma})_{\text{jump}} = 0$. Consequently the equation of motion (2.53) of the trial f_{σ} is identical to the equation of motion (2.29) of the true state f_{ρ} . The non-linearity of the equations of motion will however distort the Gaussian such that the ansatz state starts to deviate from the real state. The trajectories of (2.45) thus satisfy

$$\begin{aligned} \frac{dx}{dt} &= p - \frac{g}{4} \frac{x^2 \left(p - p_0\right)}{\sigma_p^4}, \\ \frac{dp}{dt} &= -x + \frac{g}{4} \left(\frac{x \left(p - p_0\right)^2}{\sigma_p^4} - \frac{3x}{\sigma_p^2} + x^2 \frac{x - x_0}{\sigma_x^2 \sigma_p^2} - 4x^3 \right). \end{aligned}$$

Clearly the equations of motion for the average phase space position of the state become

$$\begin{aligned} \frac{dx_0}{dt} &= p_0, \\ \frac{dp_0}{dt} &= -x_0 \left(1 + \frac{3}{4} \frac{g}{\sigma_p^2}\right) - gx_0^3, \end{aligned}$$

which for $\sigma_p \to \infty$ (i.e., $\sigma_x \to 0$) reduce to the equations of motion of the real Hamiltonian (2.54). The latter equations, including the σ_p -dependent term, express Ehrenfest's theorem [34]. The restoration of Ehrenfest's theorem is indicative of the gain made by propagating the classical trial system with the effective Hamiltonian rather than the real Hamiltonian. It should moreover be noted that, at least for the present example, the initial behavior of the distance is drastically different in both situations. Within the truncated Wigner approximation the initial distance will always increase linear in time. The slope is simply determined by the initial value of the $O(\hbar^2)$ correction to the Poisson bracket. So although the correction is of $O(\hbar^2)$, it does cause a discrepancy between the exact and the truncated distribution which increases linearly in time. The variational result however has vanishing corrections within first order, which implies that the initial increase in the distance is quadratic. The result is thus correct up to second order, i.e. up to the deviation from Gaussianity due to the non-linearity of the equations of motion. It is interesting to note that although the equation of motion for the expected phase space positions of the variational evolution is in agreement with Eherenfest's theorem, one can not directly extract the effective Hamiltonian from the theorem. One might expect, based on Eherenfest's theorem alone, that the effective Hamiltonian only contains a correction on the potential because the original Hamiltonian was harmonic in momentum but this is not the case.

The present effective Hamiltonian can be used as an ansatz effective Hamiltonian for the optimization of states that are not Gaussian. The efficiency of course greatly depends on the shape of the state but if properly parametrized the initial time evolution can never be worse than the truncated Wigner result. Moreover, first calculating the exact effective Hamiltonian for a tractable state circumvents in some way the *lack of inspiration* effect one has when directly optimizing the distance with a parametrized trial Hamiltonian. To illustrate the method we propagate the initial Gaussian Wigner function in time along the classical trajectories of the effective Hamiltonian. To construct the effective Hamiltonian we calculate the average position and momentum and the variance at each point in time. Note that this is suboptimal whenever



Figure 2.9: The Hilbert-Schmidt distance between the exact state and the approximate classical state as a function of time for the normal truncated Wigner (red dashed) and the variational truncated Wigner (full blue) approximation for g = 1/25. The orignal state was unsqueezed, i.e. $\sigma_x = \sigma_p = 1/2$, and centered around the origin $(x_0, p_0) = (0, 0)$.

the state is not Gaussian. In order to determine the goodness of the approximation we simply calculate the Hilbert-Schmidt distance between the approximate state and the exact state. The latter is calculated by a second order Suzuki-Trotter [35] expansion of the time evolution operator of the Wigner function on a rectangular phase space grid. This is essentially an improved version of the method presented in [33]. The results for q = 1/25 are depicted in Figs. (2.9) and (2.10) for two different initial states. Although the qualitative and quantitative behavior of both figures is rather different they have one thing in common. Both figures clearly show how the initial increase in the distance is quadratic for the variational result whereas the semiclassical truncated Wigner approximation has a distance which grows linear with time. Figure 2.9 moreover shows that the variational result is not necessarily better at all points in time. Two quantum jumps in the exact solution can destructively interfere such that the original truncated Wigner becomes better. This is however always a second order effect since it requires at least two jumps. This effect is clearly not incorporated in our Markovian determination of the effective Hamiltonian. Finally note that distance for the displaced wavepacket is overall an order of magnitude larger than the distance for the undisplaced wavepacket. For small q, the latter is close to the ground state of the quartic oscillator such that neither the true evolution nor the semiclassical approximations significantly alter the initial state.



Figure 2.10: The Hilbert-Schmidt distance between the exact state and the approximate classical state as a function of time for the normal truncated Wigner (red dashed) and the variational truncated Wigner (full blue) approximation for g = 1/25. The orignal state was unsqueezed, i.e. $\sigma_x = \sigma_p = 1/2$, and centered around the origin $(x_0, p_0) = (2, 0)$.

Chapter 3

Interacting subsystems

In the previous chapter we derived the phase space propagator for a single-particle system. Many interesting systems however consist of interacting subsystems. One of those subsystems is usually of particular interest. In this chapter we generalize the previous phase space description with the help of influence functionals [24], allowing to describe the behavior of the subsystem of interest, coupled with an external (quantum) system, solely in terms of its own variables. Although this can be done for arbitrary systems we focus on a single particle interacting with some bath. The general results are derived in section 3.1.

Section 3.2 describes a single particle connected to a set of harmonic oscillators such that the dynamics of the bath is analytically tractable. As an example we calculate the propagator for the reduced Wigner function associated with the Ohmic Caldeira-Legett model [25]. And we present linear response coefficients for models in which the dispersion is non Ohmic.

For non-linear coupling the resulting path integral can not be solved analytically. A perturbation theory for the propagator is developed in section 3.3. By exactly resumming this series, we find a Dyson integral equation for the reduced propagator, from which the equation of motion for the reduced Wigner function is derived. It is shown how the true self-energy for the equation of motion is connected with the influence functional for the path integral. Explicit expressions are presented in terms of the bare Wigner propagator.

In section 3.4 we consider a polaronic coupling. We show under which approximations the resulting equation of motion reduces to the Wigner-Boltzmann equation and present an alternative method to calculate the linear response coefficients of the system. The method is based on a systematic truncation of the Liouville equation for the reduced distribution function. Explicit expressions for the conductivity of the Fröhlich polaron are obtained, and the discrepancy between the Kadanoff [41] and the Feynman-Hellwarth-Iddings-Platzmann [42] mobility is elucidated.

3.1 Influence functionals in phase space

In contrast to the previous chapter consider a slightly more complicated system that consists of two subsystems with generalized coordinates x and u. Again, without loss of generality, in one dimension. The subsystems are coupled by a potential $V_I(x,u)$, which is incorporated in the action as $S_I[x, u]$. Although we could simply start from a higher dimensional version of the results obtained in the previous chapter, for clarity we will explicitly redo the calculation for the two subsystem problem starting from Feynman's path integral. The extension of the path integral (2.7) takes the form

$$K(x_b, u_b, t_b | x_a, u_a, t_a) = \int_{x(t_a) = x_a}^{x(t_b) = x_b} \int_{u(t_a) = u_a}^{u(t_b) = u_b} \mathcal{D}x \mathcal{D}u \exp\left(\frac{i}{\hbar} \left(S_x \left[x\right] + S_u \left[u\right] + S_I \left[x, u\right]\right)\right)$$
(3.1)

where $S_x[x]$ and $S_u[u]$ are the non-interacting contributions of the subsystems x and u to the action. Again, for brevity, the path variables x and u are implicitly assumed to be time dependent. If $\{|n\rangle\}$ denotes a complete orthonormal set of states for the x subsystem, and $\{|j\rangle\}$ similarly for the u subsystem, the amplitude (2.8) can be generalized to

$$A(n_b, j_b, t_b | n_a, j_a, t_a) = \iiint \langle n_b | x_b \rangle \langle j_b | u_b \rangle K(x_b, u_b, t_b | x_a, u_a, t_a) \times \langle u_a | j_a \rangle \langle x_a | n_a \rangle dx_a dx_b du_a du_b, \quad (3.2)$$

The conditional transition probability $P(n_b, j_b, t_b | n_a, j_a, t_a) = |A(n_b, j_b, t_b | n_a, j_a, t_a)|^2$ for subsystem x to go from state $|n_a\rangle$ at t_a to state $|n_b\rangle$ at t_b , while subsystem u goes from $|j_a\rangle$ to $|j_b\rangle$ thus becomes

$$P(n_b, j_b, t_b | n_a, j_a, t_a) = \iiint \iiint \langle x'_b | n_b \rangle \langle u'_b | j_b \rangle K^*(x'_b, u'_b, t_b | x'_a, u'_a, t_a) \langle j_a | u'_a \rangle \langle n_a | x'_a \rangle \times \langle n_b | x_b \rangle \langle j_b | u_b \rangle K(x_b, u_b, t_b | x_a, u_a, t_a) \langle u_a | j_a \rangle \langle x_a | n_a \rangle dx_a dx_b du_a du_b dx'_a dx'_b du'_a du'_b.$$
(3.3)

From here on we assume that only the description of subsystem x is physically relevant. In other words, one is interested in the probability $P(n_b, t_b | n_a, t_a)$ of the transition of subsystem x from state $|n_a\rangle$ to $|n_b\rangle$. This can be found from the conditional probability (3.3) by summing over all final states $|j_b\rangle$ and initial states $|j_a\rangle$, weighted by the probability that subsystem u was initially in state $|j_a\rangle$:

$$P(n_b, t_b | n_a, t_a) = \sum_{j_a, j_b} P(j_a, t_a) P(n_b, j_b, t_b | n_a, j_a, t_a).$$
(3.4)

Substitution of the conditional probability (3.3) into Eq. (3.4) and regrouping terms leads to

$$P(n_b, t_b | n_a, t_a) = \iiint \iiint \langle x'_b | n_b \rangle K^*(x'_b, u'_b, t_b | x'_a, u'_a, t_a) \langle n_b | x_b \rangle \times \\ \times \langle n_a | x'_a \rangle K(x_b, u_b, t_b | x_a, u_a, t_a) \langle x_a | n_a \rangle \times \\ \times \left\{ \sum_{j_a} \langle u_a | j_a \rangle P(j_a, t_a) \langle j_a | u'_a \rangle \right\} \left\{ \sum_{j_b} \langle u'_b | j_b \rangle \langle j_b | u_b \rangle \right\} dx_a dx_b du_a du_b dx'_a dx'_b du'_a du'_b. \quad (3.5)$$

The sum over the initial states $|j_a\rangle$ is clearly identified as the initial density matrix of subsystem u, whereas the closure relation ensures that the sum over all final states $|j_b\rangle$ reduces to $\delta(u_b - u'_b)$. Then, substitution of expression (3.1) for the propagators $K(\cdots)$ and rearranging terms one ends up with the following expression for the required transition probability:

$$P(n_b, t_b | n_a, t_a) = \iiint \langle x'_b | n_b \rangle \langle n_b | x_b \rangle \langle n_a | x'_a \rangle \langle x_a | n_a \rangle \times \\ \times \int_{x(t_a)=x_a}^{x(t_b)=x_b} \int_{x'(t_a)=x'_a}^{x'(t_b)=x'_b} \mathcal{D}x \mathcal{D}x' \exp\left(\frac{i}{\hbar} \left(S_x \left[x\right] - S_x \left[x'\right]\right)\right) \mathcal{F}\left[x, x'\right] \mathrm{d}x_a \mathrm{d}x_b \mathrm{d}x'_a \mathrm{d}x'_b, \quad (3.6)$$

with

$$\mathcal{F}[x,x'] = \iiint \rho\left(u_a, u'_a, t_a\right) \delta(u_b - u'_b) \left\{ \int_{u(t_a)=u_a}^{u(t_b)=u_b} \mathcal{D}u \exp\left(\frac{i}{\hbar} \left(S_u\left[u\right] + S_I\left[x,u\right]\right)\right) \right\} \times \left\{ \int_{u'(t_a)=u'_a}^{u'(t_b)=u'_b} \mathcal{D}u' \exp\left(\frac{-i}{\hbar} \left(S_u\left[u'\right] + S_I\left[x',u'\right]\right)\right) \right\} du_a du_b du'_a du'_b. \quad (3.7)$$
$\mathcal{F}[x, x']$ contains a double path integral as indicated by the braces, and it can be regarded as an influence functional [24] since it describes the full influence of subsystem u on subsystem x.

The relation (2.1) readily allows to write the influence functional in terms of the initial Wigner distribution function of the u system. Expressed in the center-of-mass and relative coordinate system it becomes:

$$\mathcal{F}[x,x'] = \iiint \iiint f(u_a, p_a, t_a) e^{i(p_a \eta_a - p_b \eta_b)/\hbar} \times \\ \times \int_{u(t_a)=u_a}^{u(t_b)=u_b} \int_{\eta(t_a)=\eta_a}^{\eta(t_b)=\eta_b} \mathcal{D}u \mathcal{D}\eta \exp\left\{\frac{i}{\hbar} \left(\begin{array}{c} S_u \left[u + \frac{\eta}{2}\right] + S_I \left[x, u + \frac{\eta}{2}\right] \\ -S_u \left[u - \frac{\eta}{2}\right] - S_I \left[x', u - \frac{\eta}{2}\right] \end{array}\right)\right\} \frac{\mathrm{d}p_a \mathrm{d}p_b}{2\pi\hbar} \mathrm{d}u_a \mathrm{d}\eta_a \mathrm{d}u_b \mathrm{d}\eta_b,$$

$$(3.8)$$

where a factor $\delta(\eta_b)$ was replaced by its plane wave representation.

Proceeding along the lines of the previous chapter one obtains the time evolution of the reduced density matrix of subsystem x:

$$\rho(x_b, x'_b, t_b) = \iint \mathrm{d}x_a \mathrm{d}x'_a \rho(x_a, x'_a, t_a) \times \left\{ \int_{x(t_a)=x_a}^{x(t_b)=x_b} \int_{x'(t_a)=x'_a}^{x'(t_b)=x'_b} \mathcal{D}x \mathcal{D}x' \exp\left(\frac{i}{\hbar} \left(S_x\left[x\right] - S_x\left[x'\right]\right)\right) \mathcal{F}\left[x, x'\right] \right\}, \quad (3.9)$$

which differs from (2.14) merely by the occurrence of the influence functional in the path integral.

Note that we have assumed the two subsystems to be initially independent such that the probability $P(j_a, t_a)$ of finding u in state $|j_a\rangle$ is independent of the state of x. This means that the initial total density matrix was supposed to be separable.

Some useful properties of the influence functional are listed below. The identity

$$\mathcal{F}^{*}[x, x'] = \mathcal{F}[x', x], \qquad (3.10)$$

follows directly from Eq. (3.7) by interchanging x and x'. Note that this property will later ensure that the propagator for the Wigner function is always a real quantity. Furthermore, if there are a number of statistically and dynamically independent subsystems u_j acting on xand if $\mathcal{F}^j(x, x')$ is the influence functional of the *j*th subsystem on x, then the total influence function is the product of all the individual functionals \mathcal{F}^j :

$$\mathcal{F}[x,x'] = \prod_{j=1}^{N} \mathcal{F}^{j}[x,x'].$$
(3.11)

This property is a direct consequence of the total initial density emerging as a simple product when all u_j are statistically independent. If they are also dynamically independent, then each density matrix can propagate separately. Finally, it is often convenient to write the influence functional in the form

$$\mathcal{F}[x, x'] = \exp\left(\frac{i}{\hbar}\Phi[x, x']\right)$$
(3.12)

where $\Phi[x, x']$ is called the influence phase. For independent subsystems, as follows from (3.11), the corresponding influence phases add. According to Eq. (3.10), the influence phase turns out to be antisymmetric under the exchange of x and x' if the phase is real, and symmetric if the phase is imaginary. More properties of influence functionals can be found in [24].

It follows from Eq. (3.9), and in analogy with the analysis presented in section 2.2, that the propagator for the reduced Wigner distribution function becomes

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \iint \int_{x(t_a) = x_a}^{x(t_b) = x_b} \int_{\xi(t_a) = \xi_a}^{\xi(t_b) = \xi_b} \mathcal{D}x \mathcal{D}\xi \mathcal{F}\left[x + \frac{\xi}{2}, x - \frac{\xi}{2}\right] \times \\ \times \exp\left\{\frac{i}{\hbar}\left(-p\xi|_{t_a}^{t_b} + S_x\left[x + \frac{\xi}{2}\right] - S_x\left[x - \frac{\xi}{2}\right]\right)\right\} \frac{\mathrm{d}\xi_b \mathrm{d}\xi_a}{2\pi\hbar}.$$
(3.13)

If the action of the system x is of the form

$$S_x[x] = \int_{t_a}^{t_b} \left[\frac{m}{2}\dot{x}^2 - V(x)\right] \mathrm{d}t$$

we can again simplify the propagator to:

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \frac{1}{2\pi\hbar} \int_{\substack{p(t_b) = m\dot{x}_b \\ p(t_a) = m\dot{x}_a}}^{x(t_b) = x_b} \mathcal{D}x \int \mathcal{D}\xi \mathcal{F} \left[x + \frac{\xi}{2}, x - \frac{\xi}{2} \right] \times \\ \times \exp\left\{ -\frac{i}{\hbar} \int_{t_a}^{t_b} \left[m\ddot{x}\xi + \left(V\left(x + \frac{\xi}{2}\right) - V\left(x - \frac{\xi}{2}\right) \right) \right] dt \right\}.$$
(3.14)

The crucial ingredient for further development is the influence functional $\mathcal{F}[x, x']$. Clearly representing the propagator of subsystem u under the influence of subsystem x, the path integrals in (3.7) can be calculated analytically if $S_u[u] + S_I[x,u]$ is quadratic in u. Below the results for a bare harmonic action S_u with a linear coupling S_I will be discussed in some detail.

3.2 Harmonic subsystems with linear coupling

3.2.1 A single oscillator

In this section we have reduced the subsystem u to a single harmonic oscillator with mass Mand with potential energy $V(u) = M\omega^2 u^2/2$, interacting with the subsystem x of interest. Taking the interaction energy to be $u \cdot \gamma(x)$, with an arbitrary coupling function $\gamma(x)$ and a linear dependence on u, we are left with $S_I[x, u] = -\int_{t_a}^{t_b} u\gamma_t(x) dt$, where we added a subscript t to γ to remember the time at which its path variable x should be evaluated. The total action of subsystem u, to be used in the influence functional (3.8), is thus

$$S_u[u] + S_I[x,u] = \int_{t_a}^{t_b} \left(\frac{M}{2}\dot{u}^2 - \frac{M}{2}\omega^2 u^2 - u\gamma_t(x)\right) dt.$$
(3.15)

The argument in the exponent of Eq. (3.8) thus becomes linear in η and in u:

$$\mathcal{F}[x,x'] = \iiint \iiint f(u_a, p_a, t_a) e^{i(p_a \eta_a - p_b \eta_b)/\hbar} \int_{u(t_a) = u_a}^{u(t_b) = u_b} \mathcal{D}u \exp\left\{-\frac{i}{\hbar} \int_{t_a}^{t_b} u\left[\gamma_t(x) - \gamma_t(x')\right] \mathrm{d}t\right\} \times \\ \times \int_{\eta(t_a) = \eta_a}^{\eta(t_b) = \eta_b} \mathcal{D}\eta \exp\left\{-\frac{i}{\hbar} \int_{t_a}^{t_b} \left[M\dot{u}\dot{\eta} - M\omega^2 u\eta - \eta\frac{\gamma_t(x) + \gamma_t(x')}{2}\right] \mathrm{d}t\right\} \frac{\mathrm{d}p_a \mathrm{d}p_b}{2\pi\hbar} \mathrm{d}u_a \mathrm{d}\eta_a \mathrm{d}u_b \mathrm{d}\eta_b.$$

After an integration by parts of the kinetic term $\int_{t_a}^{t_b} \dot{u}\dot{\eta}dt = \dot{u}_b\dot{\eta}_b - \dot{u}_a\dot{\eta}_a - \int_{\mathbf{t_a}}^{\mathbf{t_b}} \ddot{u}\eta dt$, and imposing $M\dot{u}_{a,b} = p_{a,b}$, the path integral over η becomes unconstrained:

$$\mathcal{F}[x,x'] = \iiint f(u_a, p_a, t_a) \int_{\substack{p(t_b) = Mu_b \\ p(t_a) = Mu_a}}^{u(t_b) = u_b} \mathcal{D}u \exp\left\{-\frac{i}{\hbar} \int_{t_a}^{t_b} \left[\gamma_t(x) - \gamma_t(x')\right] u dt\right\} \times \\ \times \int \mathcal{D}\eta \exp\left\{\frac{i}{\hbar} \int_{t_a}^{t_b} \left[-M\ddot{u} - M\omega^2 u - \frac{\gamma_t(x') + \gamma_t(x)}{2}\right] \eta dt\right\} \frac{dp_a dp_b du_a du_b}{2\pi\hbar}.$$
(3.16)

The path integral over all η restricts the phase space trajectories of u to

$$M\left(\ddot{u}+\omega^2 u\right)+\frac{\gamma_t(x)+\gamma_t(x')}{2}=0,$$
(3.17)

with the formal solution

$$u(t) = u_a \cos\left[\omega \left(t - t_a\right)\right] + \frac{\dot{u}_a}{\omega} \sin\left[\omega \left(t - t_a\right)\right] - \int_{t_a}^t \frac{\gamma_s(x) + \gamma_s(x')}{2M} \frac{\sin\left[\omega \left(t - s\right)\right]}{\omega} \,\mathrm{d}s.$$

The remaining path integral on the first line of (3.16) imposes that the initial velocity is $\dot{u}_a = p_a/M$. The trajectories in u are thus reduced to a single path, with the conditions $p_{a,b} = M\dot{u}_{a,b}$ at the end points, which also eliminate the integrations over u_b and p_b . One thus readily arrives at

$$\mathcal{F}[x,x'] = \exp\left\{\frac{i}{2\hbar M\omega} \int_{t_a}^{t_b} \int_{t_a}^{t} \left[\gamma_s(x) + \gamma_s(x')\right] \left[\gamma_t(x) - \gamma_t(x')\right] \sin\left[\omega\left(t-s\right)\right] \,\mathrm{d}s\mathrm{d}t\right\} \times \\ \times \iint f\left(u_a, p_a, t_a\right) \exp\left\{-\frac{i}{\hbar} \int_{t_a}^{t_b} \left[\begin{array}{c} u_a \cos\left[\omega\left(t-t_a\right)\right] \\ + \frac{p_a}{M\omega} \sin\left[\omega\left(t-t_a\right)\right] \end{array}\right] \left[\gamma_t(x) - \gamma_t(x')\right] \mathrm{d}t\right\} \mathrm{d}r_a \mathrm{d}p_a, \quad (3.18)$$

One might be concerned about the normalizing factors accompanying the several delta functions in the derivation, but this possible problem is resolved by considering the uncoupled limit $\gamma = 0$. An alternative derivation, using the explicit solution of the Feynman path integral [22] for the action $(S_u [u] + S_I [x, u])$, confirms this result.

Clearly the first line in expression (3.18) is independent of the initial state of the harmonic oscillator. This term represents an effective interaction of system x with itself. The second line is an expectation value which transfers all necessary information about the initial state of the harmonic u system into x.

Example: initial wave packet

Despite the classical trajectories which govern its dynamics, the influence functional (3.18) is intrinsically of quantum mechanical nature, because the initial Wigner distribution function $f(u_a, p_a, t_a)$ of the oscillator is bound to satisfy the uncertainty principle. A sharply defined initial distribution like $\delta(u_a - u_0)\delta(p_a - p_0)$ can not be of the form (2.1). However, a valid initial wave function could be a Gaussian wave packet

$$\Psi_G(u, t_a) = \frac{1}{\sqrt{\Delta\sqrt{2\pi}}} \exp\left(-\frac{(u-u_0)^2}{4\Delta^2}\right) e^{ip_0 u/\hbar}.$$

From the corresponding density matrix $\rho_G(u, u', t) = \Psi_G^*(u', t) \Psi_G(u, t)$ one easily finds the Wigner distribution function of this wave packet

$$f_G(u, p, t_a) = \frac{1}{\pi\hbar} \exp\left(-\frac{(u - u_0)^2}{2\Delta^2} - 2\Delta^2 \left(\frac{p - p_0}{\hbar}\right)^2\right).$$
 (3.19)

Then, by performing the integrations in Eq.(3.18) and rearranging some terms one finds the following influence phase (3.12):

$$\Phi_{G}[x,x'] = \frac{1}{2M\omega} \int_{t_{a}}^{t_{b}} \int_{t_{a}}^{t} \left[\gamma_{s}(x) + \gamma_{s}(x')\right] \left[\gamma_{t}(x) - \gamma_{t}(x')\right] \sin\left[\omega\left(t-s\right)\right] \,\mathrm{d}s \,\mathrm{d}t \\ - u_{0} \int_{t_{a}}^{t_{b}} \left[\gamma_{t}(x) - \gamma_{t}(x')\right] \cos\left[\omega\left(t-t_{a}\right)\right] \,\mathrm{d}t - \frac{p_{0}}{M\omega} \int_{t_{a}}^{t_{b}} \left[\gamma_{t}(x) - \gamma_{t}(x')\right] \sin\left[\omega\left(t-t_{a}\right)\right] \,\mathrm{d}t \\ + \frac{i}{4\hbar} \int_{t_{a}}^{t_{b}} \int_{t_{a}}^{t_{b}} \left[\gamma_{s}(x) - \gamma_{s}(x')\right] \left[\gamma_{t}(x) - \gamma_{t}(x')\right] \left[\begin{pmatrix} \left(\Delta^{2} + \frac{\hbar^{2}}{4\Delta^{2}M^{2}\omega^{2}}\right) \cos\omega\left(s-t\right) \\ + \left(\Delta^{2} - \frac{\hbar^{2}}{4\Delta^{2}M^{2}\omega^{2}}\right) \cos\omega\left(s+t-2t_{a}\right) \right] \,\mathrm{d}s \,\mathrm{d}t \\ (3.20)$$

The real part of the influence phase is the same as one would obtain from a (forbidden) initial Wigner distribution function $\delta(u_a - u_0)\delta(p_a - p_0)$. Besides the effective interacting of system x with itself, the real part now contains an external driving potential which oscillates in time with a frequency ω and its spatial dependence is given by $\gamma(x)$. The magnitude of this driving potential depends on the initial average (vacuum) displacement of the oscillator (u_0, p_0) . The imaginary part of the influence phase results from the uncertainty on the initial position and momentum of u; its physical significance becomes more apparent in the next example. Note that some terms vanish under specific conditions, e.g., if the average initial position or momentum are zero. The last term becomes zero whenever $\Delta^2 = \frac{\hbar}{2M\omega}$. This condition is satisfied if the oscillator was initially in an unsqueezed coherent state. In that case one finds the ground state or vacuum influence phase:

$$\Phi_{vac}\left[x,x'\right] = \frac{1}{2M\omega} \int_{t_a}^{t_b} \int_{t_a}^{t} \left[\gamma_s(x) + \gamma_s(x')\right] \left[\gamma_t(x) - \gamma_t(x')\right] \sin\left[\omega\left(t-s\right)\right] \,\mathrm{d}s\mathrm{d}t \\ + \frac{i}{4M\omega} \int_{t_a}^{t_b} \int_{t_a}^{t_b} \left[\gamma_s(x) - \gamma_s(x')\right] \left[\gamma_t(x) - \gamma_t(x')\right] \cos\left[\omega\left(s-t\right)\right] \,\mathrm{d}s\mathrm{d}t.$$
(3.21)

Example: thermal equilibrium

The case of thermal equilibrium at the start of course deserves some additional attention. The initial equilibrium Wigner function of the harmonic oscillator u is then given by

$$f_{eq}\left(u_{a}, p_{a}, t_{a}\right) = \frac{\tanh\frac{1}{2}\beta\hbar\omega}{\pi\hbar} \exp\left(-\frac{\tanh\frac{1}{2}\beta\hbar\omega}{\hbar\omega}\left(M\omega^{2}u_{a}^{2} + \frac{p_{a}^{2}}{M}\right)\right).$$
(3.22)

It follows from Eq. (3.18) that the equilibrium influence phase $\Phi_{eq}[x, x']$ is

$$\Phi_{eq}\left[x,x'\right] = \frac{1}{2M\omega} \int_{t_a}^{t_b} \int_{t_a}^{t} \left[\gamma_s(x) + \gamma_s(x')\right] \left[\gamma_t(x) - \gamma_t(x')\right] \sin\left[\omega\left(t-s\right)\right] \,\mathrm{d}s \mathrm{d}t + \frac{i \coth\left(\frac{1}{2}\beta\hbar\omega\right)}{4M\omega} \int_{t_a}^{t_b} \int_{t_a}^{t_b} \left[\gamma_t(x) - \gamma_t(x')\right] \left[\gamma_s(x) - \gamma_s(x')\right] \cos\left[\omega\left(t-s\right)\right] \,\mathrm{d}s \mathrm{d}t \quad (3.23)$$

While the real parts of Φ_{eq} and Φ_{vac} are the same, the imaginary part of Φ_{eq} has increased by a factor $\operatorname{coth}\left(\frac{\beta\hbar\omega}{2}\right)$ as compared to Φ_{vac} , as a consequence of thermal broadening of the distribution. Note now that $\operatorname{coth}\left(\frac{\beta\hbar\omega}{2}\right) = [1 + 2n_B(\omega)]$, with $n_B(\omega)$ the Bose-Einstein distribution with zero chemical potential. When the temperature is zero, system x can only interact with the zero point fluctuations of u, allowing only losses trough spontaneous emission. At finite temperature these fluctuations increase, incorporating the effects of absorption and stimulated emission. A more detailed discussion can be found in [24].

3.2.2 Many independent oscillators

The generalization of the result from one to many oscillators is trivial if the oscillators are independent. According to property (3.11) the total influence functional then becomes the product of all the individual influence functionals. Consider every oscillator u_j to have a mass M_j , a frequency ω_j and consider the interaction energy with x to be $u_j \cdot \gamma_j(x)$. Then we immediately arrive at the following expression for the total influence phase of a collection of N oscillators

$$\mathcal{F}_{N}[x,x'] = \exp\left\{\frac{i}{\hbar}\sum_{j=0}^{N}\frac{1}{2M_{j}\omega_{j}}\int_{t_{a}}^{t_{b}}\int_{t_{a}}^{t}\left[\gamma_{j}(x_{s}) + \gamma_{j}(x'_{s})\right]\left[\gamma_{j}(x_{t}) - \gamma_{j}(x'_{t})\right]\sin\left[\omega_{j}\left(t-s\right)\right]\,\mathrm{dsd}t\right\} \times \prod_{j=0}^{N}\iint f_{j}\left(u_{a},p_{a},t_{a}\right)\exp\left\{-\frac{i}{\hbar}\int_{t_{a}}^{t_{b}}\left[\begin{array}{c}u_{a}\cos\left[\omega_{j}\left(t-t_{a}\right)\right]\\+\frac{p_{a}}{M_{j}\omega_{j}}\sin\left[\omega_{j}\left(t-t_{a}\right)\right]\end{array}\right]\left[\gamma_{j}(x_{t}) - \gamma_{j}(x'_{t})\right]\,\mathrm{d}t\right\}\mathrm{d}r_{a}\mathrm{d}p_{a},$$

$$(3.24)$$

where $f_j(u_a, p_a, t_a)$ represents the initial Wigner function of the *j*th oscillator. Let us consider a tractable simple example now that can easily be generalized to more complicated situations and contains a lot of physics.

Example: Equilibrium oscillators with bilinear coupling

If we assume the interaction energy to be bilinear in $\{u_j, x\}$, such that $u \cdot \gamma_j(x) = \gamma_j u \cdot x$, and if additionally all oscillators are initially in thermal equilibrium (3.22), then the influence phase associated with influence functional (3.24) is given by

$$\Phi_{eq,N}\left[x,x'\right] = \sum_{j=0}^{N} \frac{\gamma_j^2}{2M_j\omega_j} \int_{t_a}^{t_b} \int_{t_a}^{t} \left(x_s + x'_s\right) \left(x_t - x'_t\right) \sin\left[\omega_j\left(t - s\right)\right] \,\mathrm{d}s \mathrm{d}t \\ + \sum_{j=0}^{N} \frac{i\gamma_j^2}{4M_j\omega_j} \coth\left(\frac{1}{2}\beta\hbar\omega_j\right) \int_{t_a}^{t_b} \int_{t_a}^{t_b} \left(x_t - x'_t\right) \left(x_s - x'_s\right) \cos\left[\omega_j\left(t - s\right)\right] \,\mathrm{d}s \mathrm{d}t.$$

In the continuum limit, when $N \to \infty$ while $\omega_{j+1} - \omega_j \to 0$, we can assume there is a distribution of oscillators, such that the relevant weight $\Gamma(\omega)d\omega$ of the oscillators between ω and $\omega + d\omega$ is

$$\Gamma(\omega) = \sum_{j=0}^{\infty} \frac{\gamma_j^2}{M_j \omega_j} \delta(\omega - \omega_j)$$

In this case the influence phase becomes

$$\Phi_{eq,many}\left[x,x'\right] = \frac{1}{2} \int_{t_a}^{t_b} \int_{t_a}^t \left(\int_0^\infty \Gamma(\omega) \sin\left[\omega\left(t-s\right)\right] \,\mathrm{d}\omega\right) \left(x_s + x'_s\right) \left(x_t - x'_t\right) \,\mathrm{d}s \,\mathrm{d}t \\ + \frac{i}{\hbar} \int_{t_a}^{t_b} \int_{t_a}^{t_b} \left[\int_0^\infty \left(\frac{\hbar\Gamma(\omega)}{4} \coth\frac{\beta\hbar\omega}{2}\right) \cos\left[\omega\left(t-s\right)\right] \,\mathrm{d}\omega\right] \left(x_t - x'_t\right) \left(x_s - x'_s\right) \,\mathrm{d}s \,\mathrm{d}t.$$

If x is the coordinate of an otherwise free particle with mass m, we find the following propagator for its reduced Wigner function

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \frac{1}{2\pi\hbar} \int_{\substack{x(t_a) = x_a \\ p(t_a) = m\dot{x}_a}}^{x(t_b) = x_b} \mathcal{D}x \int \mathcal{D}\xi \exp\left(-\frac{1}{\hbar^2} \int_{t_a}^{t_b} \int_{t_a}^{t_b} R(t-s)\xi_t \cdot \xi_s \mathrm{d}s\mathrm{d}t\right) \times \\ \times \exp\left(-\frac{i}{\hbar} \int_{t_a}^{t_b} \left(m\ddot{x} - \int_{t_a}^t A(t-s)x_s \mathrm{d}s\right) \cdot \xi_t \mathrm{d}t\right),$$

with A(t) and R(t) defined as:

$$A(t) = \int_0^\infty \Gamma(\omega) \sin(\omega t) d\omega,$$

$$R(t) = \int_0^\infty \frac{\hbar \Gamma(\omega)}{4} \coth\left(\frac{\beta \hbar \omega}{2}\right) \cos(\omega t) d\omega.$$

Following [18] we can further simplify the propagator by introducing an auxiliary force field F(t), defined by

$$m\ddot{x} - \int_{t_a}^t A(t-s)x_s \mathrm{d}s = F(t).$$
 (3.25)

Now one can rewrite the propagator as

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \int \mathcal{D}F \exp\left(-\frac{1}{4} \int_{t_a}^{t_b} \int_{t_a}^{t_b} F_t R^{-1}(t-s) F_s \mathrm{d}s \mathrm{d}t\right) \times \\ \times \frac{1}{2\pi\hbar} \int_{\substack{p(t_b)=m\dot{x}_b\\p(t_a)=m\dot{x}_a}}^{x(t_b)=x_b} \mathcal{D}x \int \mathcal{D}\xi \exp\left\{-\frac{i}{\hbar} \int_{t_a}^{t_b} \left[m\ddot{x} - \int_{t_a}^t A(t-s) x_s \mathrm{d}s - F(t)\right] \xi_t \mathrm{d}t\right\},$$

where we have absorbed the normalization factor in the measure $\mathcal{D}F$, and $R^{-1}(t-s)$ is the inverse functional matrix of R(t-s). The path integral in the last line is linear in ξ , such that we find

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \int \mathcal{D}F \exp\left(-\frac{1}{4} \int_{t_a}^{t_b} \int_{t_a}^{t_b} F_t R^{-1}(t-s) F_s \mathrm{d}s \mathrm{d}t\right) \times \\ \times \delta\left(x_b - x_F\left(t_b | x_a, p_a, t_a\right)\right) \delta\left(p_b - p_F\left(t_b | x_a, p_a, t_a\right)\right),$$

where $x_F(t_b|x_a, p_a, t_a)$ is the solution at time t_b of Eq. (3.25) with initial position x_a and velocity p_a/m at time t_a and p_F is its conjugate momentum. Hence the reduced Wigner function propagator can be written as the force dependent expectation value of the phase space trajectories generated by the stochastic differential equation (3.25)

$$K_{w}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a}) = \left\langle \delta\left(x_{b} - x_{F}\left(t_{b}|x_{a}, p_{a}, t_{a}\right)\right) \delta\left(p_{b} - p_{F}\left(t_{b}|x_{a}, p_{a}, t_{a}\right)\right) \right\rangle_{F}, \qquad (3.26)$$

where

$$\langle F_t \rangle_F = 0$$
, and $\langle F_t F_s \rangle_F = 2R(t-s)$.

Example: Caldeira-Legett model and thermalization

In the specific case that $\Gamma(\omega) = \eta \omega/\pi$, as considered in detail by Caldeira and Leggett in [25], we obtain $A(t) = -\eta \delta'(t)$. If additionally the temperature T_b is high enough such that we can approximate $\left[\frac{\hbar\eta\omega}{4\pi} \coth\left(\frac{\beta\hbar\omega}{2}\right)\right] \approx \frac{\eta}{2\pi\beta} + \mathcal{O}(\beta)$, we find $R(t) = \eta k T_b \delta(t-s)$. Therefore we arrive [36] at the following expression for the propagator in the high temperature limit

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \frac{1}{2\pi\hbar} \int_{\substack{p(t_b) = m\dot{x}_b \\ p(t_a) = m\dot{x}_a}}^{x(t_b) = x_b} \mathcal{D}x \int \mathcal{D}\xi \exp\left(-\frac{\eta kT_b}{\hbar^2} \int_{t_a}^{t_b} \xi_t^2 dt\right) \times \\ \times \exp\left(-\frac{i}{\hbar} \int_{t_a}^{t_b} (m\ddot{x} + \eta \dot{x}) \cdot \xi_t dt\right).$$

The ξ path integral is Gaussian and can be done, yielding

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \int_{\substack{p(t_b) = m\dot{x}_b \\ p(t_a) = m\dot{x}_a}}^{x(t_b) = x_b} \mathcal{D}x \exp\left(-\frac{1}{4\eta k T_b} \int_{t_a}^{t_b} (m\ddot{x} + \eta\dot{x})^2 \,\mathrm{d}t\right).$$

If we are not interested in the real space motion of x, for example because the initial distribution of the particle is homogeneous in space, but only in the marginal propagator $K_w(p_b, t_b|p_a, t_a)$ to go from p_a to p_b , then we get

$$K_w(p_b, t_b | p_a, t_a) = \int_{p(t_a)=p_a}^{p(t_b)=p_b} \mathcal{D}p \exp\left(-\frac{1}{2\eta k T_b} \int_{t_a}^{t_b} \left(\frac{(\dot{p})^2}{2} + \left(\frac{\eta}{m}\right)^2 \frac{p^2}{2} + \frac{\eta}{m} \dot{p}p\right) dt\right)$$

An integration by parts shows that the term in $\dot{p}p$ only contributes at the boundaries:

$$K_w(p_b, t_b | p_a, t_a) = \exp\left(-\frac{p_b^2 - p_a^2}{4mkT_b}\right) \int_{p(t_a) = p_a}^{p(t_b) = p_b} \mathcal{D}p \exp\left(-\frac{1}{2\eta kT_b} \int_{t_a}^{t_b} \left(\frac{(\dot{p})^2}{2} + \left(\frac{\eta}{m}\right)^2 \frac{p^2}{2}\right) \mathrm{d}t\right),$$

The remaining path integral is a simple Gaussian Feynman path integral. This path integral can be solved with standard techniques which yield the following expression for the reduced momentum distribution propagator:

$$K_w\left(p_b, t_b | p_a, t_a\right) = \frac{1}{\sqrt{2\pi m k T_e}} \exp\left(-\frac{1}{2m} \frac{\left(p_b - p_a \exp\left(-\frac{\eta}{m} \left(t_b - t_a\right)\right)\right)^2}{k T_e}\right),$$

where the effective temperature T_e of the particle x is given by

$$T_e = T_b \left(1 - \exp\left(-\frac{2\eta}{m} \left(t_b - t_a\right)\right) \right),$$

such that the system thermalizes with a characteristic time $\tau = \frac{m}{\eta}$. Note that the maximal transition probability is, as expected, attained along the solution of the classical equation of motion $\dot{p} + \frac{\eta}{m}p = 0$, i.e. when $p_b = p_a \exp\left(-\frac{\eta}{m}(t_b - t_a)\right)$. Finally consider the time $t_b - t_a \gg \tau$, such that the system is thermalized and $T_e \approx T_b$, then the propagator becomes

$$\lim_{(t_b-t_a)\to\infty} K_w\left(p_b, t_b | p_a, t_a\right) = \frac{1}{\sqrt{2\pi m k T_b}} \exp\left(-\frac{1}{k T_b} \frac{p_b^2}{2m}\right).$$

This means that the reduced Wigner function of the particle equilibrates into a Maxwell-Boltzmann distribution, regardless of its initial Wigner distribution.

Example: Linear response coefficient

In the previous example we solved the full propagator for the Ohmic Caldeira-Leggett model by standard path integration. Although formally possible for any linear model it becomes quite cumbersome whenever the model is not Ohmic, i.e. when the noise R(t) is correlated. If we only wish to find some expectation values it is better to adopt the stochastic differential equation approach. For instance, consider the case where we add a real driving force eE(t) to the particle, i.e. the bare action is given by

$$S_x[x] = \int_{t_a}^{t_b} \left(\frac{m}{2}\dot{x}^2 + eE(t)x\right) \mathrm{d}t,$$

consequently $\langle F_t \rangle_F = eE(t)$. It follows from expression (3.26) and Eq. (3.25) that the expected phase space position at some time t satisfies

$$m \langle \dot{x} \rangle = \langle p \rangle$$
 and $\langle \dot{p} \rangle - \int_{t_a}^t A(t-s) \langle x(s) \rangle ds = eE(t).$

If we consider the initial state to be homogeneous and in equilibrium such that $\langle x_a \rangle = \langle p_a \rangle = 0$, then we can define the current density at time t as

$$J(t) = n_0 \frac{\langle \dot{p} \rangle}{m},$$

where $n_0 = 1/V$ is the particle density. This allows us to extract the conductivity of the system, defined as the linear response coefficient

$$J(t) \equiv \int_{t_a}^t \sigma(t-s)E(s)\mathrm{d}s, \qquad (3.27)$$

from the equations of motion for the expected phase space point. The definition (3.27) of the conductivity thus yields the following relation between the Laplace transform $\mathcal{L}(\sigma, \Omega)$ of the conductivity and the Laplace transform $\mathcal{L}(A, \Omega)$ of the susceptibility

$$\mathcal{L}(\sigma,\Omega) = \frac{n_0 e^2}{m} \frac{1}{\Omega - \frac{\mathcal{L}(A,\Omega)}{m\Omega}}.$$
(3.28)

Consequently for the Ohmic Caldeira-Legget model $\mathcal{L}(A, \Omega) = -\eta s$, and we obtain

$$\mathcal{L}\left(\sigma,\Omega\right) = \frac{n_0 e^2}{m} \frac{1}{\Omega + \frac{\eta}{m}},$$

From the previous example we know that the classical Green function for the momentum has to be $\propto \exp\left(-\frac{\eta}{m}(t_b - t_a)\right)$ which is indeed proportional to the inverse Laplace transform of the conductivity obtained here. We therefore recover the expected result for the Ohmic model. The present approach however works for any other spectral function $\Gamma(\omega)$. Although one can in principle conceive any spectral function for these bilinearly coupled systems, such systems are rarely realized in nature. This however does not mean that the present discussion is useless. Not only does the Ohmic Caldeira-Leggett model provide a minimal model for dissipation in quantum mechanics, we can also regard the generic bilinear coupled system as an approximate, linearized, generic polaron model. Indeed, for the polaron the different independent oscillators j are labeled by their wave vector **k** and the coupling is given by

$$\gamma_i = \gamma(k) \exp(-i\mathbf{k} \cdot \mathbf{x})$$

For more details I refer to the next section. Although this is a non-linear function of the system variable, we can expand it for small k

$$\gamma_i \approx \gamma(k) - i\gamma(k)\mathbf{k}\cdot\mathbf{x}$$

The first term just shifts the oscillator and we can neglect or remove it by introducing a regulating field. This linearization can also be recognized as a dipole approximation. It is important to note that in such an approximation, all recoil effects caused by the $\exp(-i\mathbf{k}\cdot\mathbf{x})$ term are absent. The modification of the result due to this effect will be the topic of section 3.4. The effective coupling for the linear polaron model becomes $\gamma_j \propto k\gamma(k)$. In condensed matter theory the oscillators typically represent phonons and the system of interest is usually an

Type	$\Gamma(\omega)$	$rac{\mathcal{L}(A,\Omega)}{\Omega}$
Optical Fröhlich	$\eta\delta(\omega-\omega_{LO})$	$\eta \frac{\omega_{LO}}{\Omega(\Omega^2 + \omega_{LO})}$
Acoustic	$\eta \omega^5/\pi$	$-\eta \Omega^4$
Acoustic piezoelectric	$\eta\omega^3/\pi$	$\eta \Omega^2$

Table 3.1: Table of linear polaron model susceptibilities

electron traveling trough the lattice. For the most common cases the electron-phonon coupling is well known. I've listed three important examples, together with their Laplace transformed susceptibility in table 3.1. All examples assume the system is 3 dimensional. All of the physical constants involved in each of the problems have been absorbed in the η which represents the effective coupling of the linear model. The linear model conductivity can directly be obtained from (3.28), from which one can immediately extract the (long wavelength) optical absorption coefficient [38]

$$\Lambda(\omega) = \frac{Z_0}{n} \lim_{\epsilon \to 0^+} \operatorname{Re}\left[\mathcal{L}(\sigma, \epsilon + i\omega)\right], \qquad (3.29)$$

where n is the refractive index and $Z_0 = (\epsilon_0 c)^{-1}$ is the impedance of free space. The limit of $\epsilon \to 0^+$ is necessary because there might be poles on the imaginary axis. The absorption, for the polarons listed in table 3.1, is depicted in Fig. (3.1). Delta functions are shown as vertical arrows. For the optical Fröhlich polaron, the linear model absorption is a delta function at a frequency $\omega > \omega_{LQ}$. The frequency shift is simply caused by the interaction between the electron and the phonons and scales with the coupling. Note that the linearized optical polaron model is identical to Feynman's linear polaron model [39]. In contrast to the optical polaron, both acoustic polaron absorptions are spread over a much wider frequency range. This is related to the dispersion of the phonons. In the optical case all phonons have the same frequency $\omega = \omega_{LO}$ but the acoustic modes have a linear dispersion $\omega = ck$, where c is the speed of sound. The difference between the piezoelectric and the normal acoustic phonon can be explained by looking at the coupling. For the piezoelectric polaron the coupling scales like $\propto 1/\sqrt{k}$ whereas the acoustic phonon couples to the electron $\propto \sqrt{k}$. Consequently the coupling becomes vanishingly small for small k in the acoustic polaron, and the piezoelectric polaron coupling diverges. The effect is clearly visible in Fig. (3.1). Whereas the maximum absorption for the piezoelectric polaron occurs at $\omega = 0$, the maximum absorption for the acoustic polaron occurs at a non-zero frequency. I finally draw the attention to the fact that both acoustic polarons have a delta function in the origin. This implies that part of the linear model response is free particle like. The presence of this delta function can directly be argued from the nature of the coupling. Recall that for the piezoelectric and the acoustic polaron the coupling respectively scales like ω^3 and ω^5 such that the real time susceptibility A(t) becomes the third and fifth derivative of a delta function respectively. It follows from Eq. (3.25) that in the absence of a force particles moving at some velocity do not change their velocity. Moreover note that the piezoelectric susceptibility actually generates a force proportional to the derivative of the acceleration or the jerk. This is the acoustic analog of the Abraham–Lorentz force in semiclassical electromagnetic radiation. In the Ohmic Caldeira-Leggett model the coupling scales $\propto \omega$. This generated a susceptibility which breaks Galilei invariance and thus it generates friction. As described in the previous example the velocity of a particle will exponentially decay with a rate determined by the coupling. One can check that, apart from some relabeling, the only difference between the Ohmic model and the linearized piezoelectric polaron is precisely the delta function peak in the origin.

This curious fact signals a problem. Since both spectra are equal, apart from a delta function



Figure 3.1: Linear model optical absorption for the optical, acoustic and piezoelectric polaron. The vertical arrows represent Dirac delta functions. For the optical polaron $\omega_{LO} = 1$, and $\eta = 1$ for all three graphs.

in the origin, one of both has to violate the f-sum rule

$$\frac{m}{n_0 e^2} \int_{-\infty}^{\infty} \lim_{\epsilon \to 0^+} \operatorname{Re} \left[\mathcal{L}(\sigma, \epsilon + i\omega) \right] d\omega = \pi.$$

Since the absorption of the Ohmic model is Lorentzian the integral can easily be done and it indeed yields π . For the piezoelectric model the sum rule is violated and one finds 2π : one π from the same Lorentzian distribution and the other π from the delta function. For the normal acoustic polaron model one finds that the integral results in $4\pi/3$ where $\pi/3$ comes from the continuous part and another π from the delta function. Again the sum rule is violated but this time it can not be fixed by simply removing the delta function completely.

The sum rule does not tell us how to fix the problem. It ought to be clear, however, that the sharp resonance peaks are most sensitive to any change in the physics of the system. One would for example expect they are sensitive to including higher order, non-linear, terms in the expansion of the coupling. Indeed, within the linear model the width of the peaks does not depend on the temperature, nor does any other feature in the absorption. This is due to the linearity of the system. The fluctuations, included in R(t), are decoupled from any quantity which is linear in the phase space position.

In that respect consider the optical Fröhlich polaron, which in some sense is the most extreme case because it only has a delta function as response. Moreover, it is the best studied system. A prominent approach to study the response of this system was proposed by Feynman *et al.* [42] (hereafter referred to as FHIP) and the optical absorption based on this approach was calculated by Devreese *et al.* [38] 10 years later. The basic approach in FHIP is to expand the action around Feynman's linear polaron model and treat the difference as a perturbation. Consequently the zeroth order absorption is exactly the result shown in Fig. (3.1). Including the first order correction indeed drastically changes the result as it even removes the delta function [38]. All of this clearly shows that, although they provide great insight, one has to be extremely careful in interpreting the results of these linearized Caldeira-Leggett type of models. For more realistic non-linear coupling the resulting path integral can however not be solved. Appropriate approximation methods need to be developed such as the ones described in the previous chapter.

3.3 Perturbation theory

In analogy with section 2.4 let us construct the perturbation series for the Wigner propagator with an influence functional

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \frac{1}{2\pi\hbar} \int_{\substack{x(t_a) = x_a \\ p(t_a) = m\dot{x}_a}}^{x(t_b) = x_b} \mathcal{D}x \int \mathcal{D}\xi \exp\left(-\frac{i}{\hbar}S_0[x, \xi] + \frac{i}{\hbar}\Phi\left[x + \xi/2, x - \xi/2\right]\right)$$

where $S_0[x,\xi]$ is the bare action for the propagator in absence of any other system and where Φ is the influence phase caused by the interactions with the bath. If the bath was initially in thermal equilibrium, these influence phase is of the form

$$\frac{i}{\hbar}\Phi\left[x+\xi/2, x-\xi/2\right] = \int_{t_a}^{t_b} \int_{t_a}^{\tau_2} g(x_{\tau_1}, x_{\tau_2}, \xi_{\tau_1}, \xi_{\tau_2}) \mathrm{d}\tau_1 \mathrm{d}\tau_2, \tag{3.30}$$

which follows from expression (3.23). Recall that the subindex indicates the time at which the variables must be evaluated. Clearly the above path integral is difficult to solve as g is in general a non-linear function of both x and ξ and it contains non-local terms in time. Hence we proceed by expanding the propagator in a Taylor series around g = 0, i.e. around the free system result,

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \frac{1}{2\pi\hbar} \int_{\substack{p(t_b) = m\dot{x}_b \\ p(t_a) = m\dot{x}_a}}^{x(t_b) = x_b} \mathcal{D}x \int \mathcal{D}\xi \exp\left(-\frac{i}{\hbar}S_0[x,\xi]\right) \times \left[\sum_n \frac{\left(\int_{t_a}^{t_b} \int_{t_a}^{\tau_2} g(x_{\tau_1}, x_{\tau_2}, \xi_{\tau_1}, \xi_{\tau_2}) \mathrm{d}\tau_1 \mathrm{d}\tau_2\right)^n}{n!}\right].$$

Consider now in more detail the expression for the first order correction n = 1

$$K_{1}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a}) = \int_{t_{a}}^{t_{b}} \mathrm{d}\tau_{2} \int_{t_{a}}^{\tau_{2}} \mathrm{d}\tau_{1} \frac{1}{2\pi\hbar} \int_{\substack{p(t_{a})=x_{a}\\p(t_{a})=m\dot{x}_{a}}}^{x(t_{b})=x_{b}} \mathcal{D}x \int \mathcal{D}\xi \exp\left(-\frac{i}{\hbar}S_{0}[x,\xi]\right) \times g(x_{\tau_{1}}, x_{\tau_{2}}, \xi_{\tau_{1}}, \xi_{\tau_{2}}).$$

Now we use the Fourier representation of g, i.e.

$$g(x_{\tau_1}, x_{\tau_2}, \xi_{\tau_1}, \xi_{\tau_2}) = \iint g'(x_{\tau_1}, x_{\tau_2}, p, p') \exp\left(\frac{i}{\hbar} \left(p \cdot \xi_{\tau_1} + p' \cdot \xi_{\tau_2}\right)\right) dp dp',$$

to arrive at the following expression for K_1

$$K_{1}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a}) = \int_{t_{a}}^{t_{b}} \mathrm{d}\tau_{2} \int_{t_{a}}^{\tau_{2}} \mathrm{d}\tau_{1} \iint \mathrm{d}p \mathrm{d}p' \frac{1}{2\pi\hbar} \int_{\substack{p(t_{a})=x_{b}\\p(t_{a})=m\dot{x}_{b}}}^{x(t_{b})=x_{b}} \mathcal{D}x \int \mathcal{D}\xi g'(x_{\tau_{1}}, x_{\tau_{2}}, p, p') \\ \times \exp\left\{-\frac{i}{\hbar} \left(S_{0}[x, \xi] - \int_{t_{a}}^{t_{b}} \left[p\delta(t-\tau_{1}) + p'\delta(t-\tau_{2})\right]\xi_{t} \mathrm{d}t\right)\right\}.$$



Figure 3.2: Diagramatic representation of the perturbation series for the Wigner propagator of a system connected to a bath.

Clearly the additional terms in the action will again cause momentum jumps. In contrast to the results in the previous chapter the first order correction has two momentum jumps: one of magnitude p and one p' at times τ_1 and τ_2 respectively. If we furthermore make use of the fact that the zeroth order propagator satisfies the Chapman-Kolmogorov equation or composition rule then we directly arrive at

$$K_{1}(x_{b}, p_{b}, t_{b}|x_{a}, p_{a}, t_{a}) = \int_{t_{a}}^{t_{b}} \mathrm{d}\tau_{2} \int_{t_{a}}^{\tau_{2}} \mathrm{d}\tau_{1} \iint \mathrm{d}p \mathrm{d}p' \iint \mathrm{d}x_{2} \mathrm{d}p_{2} \iint \mathrm{d}x_{1} \mathrm{d}p_{1}g'(x_{1}, x_{2}, p, p')$$
$$\times K_{0}(x_{b}, p_{b}, t_{b}|x_{2}, p_{2}, \tau_{2}) K_{0}(x_{2}, p_{2} - p', \tau_{2}|x_{1}, p_{1} + p, \tau_{1}) K_{0}(x_{1}, p_{1}, \tau_{1}|x_{a}, p_{a}, t_{a}).$$

Now we define

$$\Sigma(x_2, p_2, \tau_2 | x_1, p_1, \tau_1) = \iint dp dp' g'(x_1, x_2, p, p') K_0(x_2, p_2 - p', \tau_2 | x_1, p_1 + p, \tau_1), \quad (3.31)$$

such that

$$K_1(x_b, p_b, t_b | x_a, p_a, t_a) = \int_{t_a}^{t_b} \mathrm{d}\tau_2 \int_{t_a}^{\tau_2} \mathrm{d}\tau_1 \iint \mathrm{d}x_2 \mathrm{d}p_2 \iint \mathrm{d}x_1 \mathrm{d}p_1 K_0(B|2) \Sigma(2|1) K_0(1|A),$$

where we have introduced the following short hand notation $J = \{x_j, p_j, \tau_j\}$. Exactly the same procedure can be repeated for the subsequent order terms in the perturbation series. The n^{th} order in the series will have 2n + 1 zeroth order propagators K_0 and n times g'. One thus constructs n self energies Σ which leave n + 1 zeroth order propagators K_0 to connect all self energies. Time ordering all the unordered time integrals will exactly cancel the n! term in the denominator. Such a structure immediately gives rise to a recurrence relation, this time in Σ instead of Γ as in chapter 2. This results in the following integral equation for the propagator

$$K_w(B|A) = K_0(B|A) + \int_{t_a}^{t_b} \mathrm{d}\tau_2 \int_{t_a}^{\tau_2} \mathrm{d}\tau_1 \iint \mathrm{d}x_2 \mathrm{d}p_2 \iint \mathrm{d}x_1 \mathrm{d}p_1 K_0(B|2) \Sigma(2|1) K_w(1|A),$$
(3.32)

as schematically depicted in Fig. (3.2). This constitutes the main result of this section. Before we finally turn our attention to the expression for the self-energy, we derive the Liouville equation from the integral equation above, which generalizes Eq. (2.29) to systems connected to a bath. Since K_0 is just the bare propagator associated with the bare action $S_0[x,\xi]$, it satisfies the Wigner-Liouville equation (2.29)

$$\frac{\partial K_0\left(B|A\right)}{\partial t_b} = \{H(B), K_0\left(B|A\right)\}_M.$$

Differentiating Eq. (3.32) with respect to the final time t_b yields

$$\frac{\partial}{\partial t_b} K_w \left(B|A \right) = \frac{\partial}{\partial t_b} K_0 \left(B|A \right) + \int_{t_a}^{t_b} \mathrm{d}\tau_2 \int_{t_a}^{\tau_2} \mathrm{d}\tau_1 \iint \mathrm{d}x_2 \mathrm{d}p_2 \iint \mathrm{d}x_1 \mathrm{d}p_1 \frac{\partial}{\partial t_b} K_0 \left(B|2 \right) \Sigma(2|1) K_w \left(1|A \right) \\ + \int_{t_a}^{\tau_2} \mathrm{d}\tau_1 \iint \mathrm{d}x_2 \mathrm{d}p_2 \iint \mathrm{d}x_1 \mathrm{d}p_1 K_0 \left(B|x_2, p_2, t_b \right) \Sigma(x_2, p_2, t_b|1) K_w \left(1|A \right).$$

In the last line we now find a propagator where the initial and final times are equal. By definition of the propagator this yields

$$K_0(B|x_2, p_2, t_b) = \delta(x_b - x_2)\delta(p_b - p_2)$$

Next we can replace the time derivatives of the zeroth order propagator by Moyal brackets and we can integrate out the delta function which yields

$$\begin{aligned} \frac{\partial}{\partial t_b} K_w \left(B|A \right) &= \left\{ H(x_b, p_b, t_b), K_0 \left(B|A \right) \right\}_M \\ &+ \left\{ H(x_b, p_b, t_b), \int_{t_a}^{t_b} \mathrm{d}\tau_2 \int_{t_a}^{\tau_2} \mathrm{d}\tau_1 \iint \mathrm{d}x_2 \mathrm{d}p_2 \iint \mathrm{d}x_1 \mathrm{d}p_1 K_0 \left(B|2 \right) \Sigma(2|1) K_w \left(1|A \right) \right\}_M \\ &+ \int_{t_a}^{t_b} \mathrm{d}\tau_1 \iint \mathrm{d}x_1 \mathrm{d}p_1 \Sigma(B|1) K_w \left(1|A \right). \end{aligned}$$

Since Moyal brackets are additive, the sum of the second arguments in the Moyal bracket is exactly equal to the right hand side of Eq. (3.32), such that we find

$$\frac{\partial}{\partial t_b} K_w(B|A) - \{H(x_b, p_b, t_b), K_w(B|A)\} = \int_{t_a}^{t_b} \mathrm{d}\tau_1 \iint \mathrm{d}x_1 \mathrm{d}p_1 \Sigma(B|1) K_w(1|A).$$
(3.33)

If we multiply the expression with the initial reduced Wigner function and integrate over (x_a, p_a) we find the equation of motion for the reduced Wigner function

$$\frac{\partial}{\partial t_b} f(B) - \{H(x_b, p_b, t_b), f(B)\} = \int_{t_a}^{t_b} \mathrm{d}\tau_1 \iint \mathrm{d}x_1 \mathrm{d}p_1 \Sigma(B|1) f(1).$$

At this point it is safe to take the limit of $t_a \to -\infty$, such that the assumption of an initial product state of bath and particle was infinitely long ago. Defining the retarded self-energy as

$$\Sigma_R(2|1) = \Theta(t_2 - t_1)\Sigma(2|1),$$

we finally arrive at the quantum Liouville equation

$$\frac{\partial}{\partial t}f(x,p,t) - \{H(x,p,t), f(x,p,t)\}_M = \iiint dt' dx' dp' \Sigma_R(x,p,t|x',p',t') f(x',p',t'). \quad (3.34)$$

This equation is the generalization of Eq. (2.29). Note that it only differs from the latter by the self energy term on the right hand side. One can show by combining its definition (3.31) and expression (3.18) for the general influence functional that

$$\int \mathrm{d}p\Sigma_R\left(x, p, t | x', p', t'\right) = 0,$$

which implies that the quantum Liouville equation satisfies the continuity equation. By doing the integral over p one can do the integral over p' in expression (3.31) which results in a delta function containing $\xi_{\tau_2} = \xi_t = 0$. Since every term in the influence phase has a component which depends on $\gamma(x_t + \xi_t/2) - \gamma(x_t - \xi_t/2)$, it vanishes whenever $\xi_t = 0$, which proves the previous equality.

As a final remark I would like to note that different resummation schemes are possible because the self-energy Σ_R also contains a propagator. One can for example also rewrite the problem in terms of an integral equation for the self-consistent self energy. This freedom even allows one to iterate over both in a similar way as the *GW*-approximation in electron gas theory.

Further results of course depend on the specifics of the system at hand. Let us focus on polaron problem.

3.4 Generic polaron response

Consider the following generic polaron Hamiltonian

$$H = H_0(\mathbf{x}, \mathbf{p}) + \sum_k \hbar \omega_k \left(b_k^{\dagger} b_k + \frac{1}{2} \right) + \sum_k \left(\gamma \left(k \right) \exp\left(-i\mathbf{k} \cdot \mathbf{x} \right) b_k^{\dagger} + \gamma^* \left(k \right) \exp\left(i\mathbf{k} \cdot \mathbf{x} \right) b_k \right),$$
(3.35)

where (\mathbf{x}, \mathbf{p}) represent the electron coordinate and momentum operator. It is coupled to some bosonic field $b_{\mathbf{k}}$ in a isotropic translational invariant way, i.e. $\gamma(k) = \gamma(|\mathbf{k}|) = \gamma(|\mathbf{k}|)$. Also the phonon frequency $\omega_k = \omega_{|\mathbf{k}|}$ is isotropic. Here $H_0(\mathbf{x}, \mathbf{p})$ is the bare Hamiltonian of the particle in absence of the bosonic field. Representing the bosonic bath operators in terms of harmonic oscillator ladder operators directly turns the action associated with Hamiltonian (3.35) into the form discussed in the previous section. The only difference is that this time the bath also couples to the momentum of the particle. A much shorter direct derivation can be done by using coherent state Wigner functions for the bath presented in the next chapter. Either way, after some straightforward albeit cumbersome algebra one arrives at the following expression for the influence phase

$$\Phi\left[\mathbf{x} + \boldsymbol{\xi}/2, \mathbf{x} - \boldsymbol{\xi}/2\right] = \sum_{k} \frac{4\left|\gamma(k)\right|^{2}}{\hbar} \int_{t_{a}}^{t_{b}} \int_{t_{a}}^{t} \sin(\mathbf{k} \cdot (\mathbf{x}_{s} - \mathbf{x}_{t})) \sin\left(\frac{\mathbf{k} \cdot \boldsymbol{\xi}_{t}}{2}\right) \cos\left(\frac{\mathbf{k} \cdot \boldsymbol{\xi}_{s}}{2}\right) \sin(\omega_{k} [t - s]) ds dt + i \sum_{k} \frac{\coth\left(\frac{\beta\hbar\omega_{k}}{2}\right)}{2} \frac{4\left|\gamma(k)\right|^{2}}{\hbar} \int_{t_{a}}^{t_{b}} \cos(\mathbf{k} \cdot (\mathbf{x}_{s} - \mathbf{x}_{t})) \sin\left(\frac{\mathbf{k} \cdot \boldsymbol{\xi}_{t}}{2}\right) \sin\left(\frac{\mathbf{k} \cdot \boldsymbol{\xi}_{s}}{2}\right) \cos(\omega_{k} [t - s]) ds dt,$$
(3.36)

for the system connected to the bosonic field if the field was originally in thermal equilibrium. Time ordering of the last term removes the factor 1/2 and brings the influence phase in the desired form (3.30), which allows to extract $g(\mathbf{x}_t, \mathbf{x}_s, \boldsymbol{\xi}_t, \boldsymbol{\xi}_s)$ from the previous expression for Φ . From definition (3.31) one arrives by straightforward algebra at the final expression for the self-energy

$$\Sigma_{R}(\mathbf{x}, \mathbf{p}, t | \mathbf{x}', \mathbf{p}', t') = \Theta(t - t') \sum_{k} \frac{2 |\gamma(k)|^{2}}{\hbar^{2}} \begin{bmatrix} n_{B}(\omega_{k}) \cos\left(\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}') - \omega_{k} (t - t')\right) \\ + (n_{B}(\omega_{k}) + 1) \cos\left(\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}') + \omega_{k} (t - t')\right) \end{bmatrix} \times \\ \times \left[K_{0}\left(\mathbf{x}, \mathbf{p} - \frac{\hbar \mathbf{k}}{2}, t | \mathbf{x}', \mathbf{p}' + \frac{\hbar \mathbf{k}}{2}, t'\right) - K_{0}\left(\mathbf{x}, \mathbf{p} + \frac{\hbar \mathbf{k}}{2}, t | \mathbf{x}', \mathbf{p}' + \frac{\hbar \mathbf{k}}{2}, t'\right) \right]. \quad (3.37)$$

One readily identifies the scattering terms associated with emission and absorption of quanta from the reservoir. Unlike in the Caldeira-Leggett model we already see that events organize themselves in terms of emission and absorption rather than self-interaction and fluctuations.

3.4.1 The Wigner-Boltzmann equation

As an important example, consider the bare system to be free, i.e. $H_0 = \mathbf{p}^2/2m$. Since the problem is harmonic its Wigner propagator is determined by the classical trajectory

$$K_0(\mathbf{x}, \mathbf{p}, t | \mathbf{x}', \mathbf{p}', t') = \delta(\mathbf{p} - \mathbf{p}')\delta\left(\mathbf{x} - \left(\mathbf{x}' + \frac{\mathbf{p}'}{m}(t - t')\right)\right).$$

Note that for a bare free particle both the bare and the total Hamiltonian of system and bath are translational invariant. Let us therefore consider the initial reduced Wigner function of the system to be translational invariant too, i.e. $f_0(\mathbf{x}, \mathbf{p}) = f(\mathbf{p})$. Under these conditions the Liouville equation (3.34) for the reduced Wigner function becomes

$$\frac{\partial}{\partial t}f\left(\mathbf{p},t\right) = \sum_{k} \frac{2\left|\gamma(k)\right|^{2}}{\hbar^{2}} \int_{-\infty}^{t} \mathrm{d}s \left[\begin{array}{c} n_{B}(\omega_{k})\cos\left(E_{+}\left(\mathbf{p},\mathbf{k},\omega_{k}\right)\left(t-s\right)/\hbar\right) \\ +\left(n_{B}(\omega_{k})+1\right)\cos\left(E_{-}\left(\mathbf{p},\mathbf{k},\omega_{k}\right)\left(t-s\right)/\hbar\right) \end{array} \right] f\left(\mathbf{p}+\hbar\mathbf{k},s\right)$$
$$-\sum_{k} \frac{2\left|\gamma(k)\right|^{2}}{\hbar^{2}} \int_{-\infty}^{t} \mathrm{d}s \left[\begin{array}{c} n_{B}(\omega_{k})\cos\left(E_{-}\left(\mathbf{p},\mathbf{k},\omega_{k}\right)\left(t-s\right)/\hbar\right) \\ +\left(n_{B}(\omega_{k})+1\right)\cos\left(E_{+}\left(\mathbf{p},\mathbf{k},\omega_{k}\right)\left(t-s\right)/\hbar\right) \end{array} \right] f\left(\mathbf{p},s\right), \quad (3.38)$$

where we introduced $E_{\pm}(\mathbf{p}, \mathbf{k}, \omega_k) = \frac{(\mathbf{p} + \hbar \mathbf{k})^2}{2m} - \frac{\mathbf{p}^2}{2m} \pm \hbar \omega_k$ for notational simplicity. Consequently, any stationary solution of the Liouville equation should satisfy

$$\sum_{k} \frac{2\pi |\gamma(k)|^{2}}{\hbar} \begin{bmatrix} n_{B}(\omega_{k})S_{+}\left(\mathbf{p},\mathbf{k},\omega_{k}\right) \\ + \left(n_{B}(\omega_{k})+1\right)S_{-}\left(\mathbf{p},\mathbf{k},\omega_{k}\right) \end{bmatrix} f\left(\mathbf{p}+\hbar\mathbf{k}\right) = \\ \sum_{k} \frac{2\pi |\gamma(k)|^{2}}{\hbar} \begin{bmatrix} n_{B}(\omega_{k})S_{-}\left(\mathbf{p},\mathbf{k},\omega_{k}\right) \\ + \left(n_{B}(\omega_{k})+1\right)S_{+}\left(\mathbf{p},\mathbf{k},\omega_{k}\right) \end{bmatrix} f\left(\mathbf{p}\right), \quad (3.39)$$

with

$$S_{\pm}(\mathbf{p},\mathbf{k},\omega_k) = \int_{-\infty}^t \frac{\mathrm{d}s}{\pi\hbar} \cos\left(E_{\pm}(\mathbf{p},\mathbf{k},\omega_k)(t-s)/\hbar\right) = \delta\left(\frac{\left(\mathbf{p}+\hbar\mathbf{k}\right)^2}{2m} - \frac{\mathbf{p}^2}{2m} \pm \hbar\omega_k\right).$$

Clearly the transition rates are now determined by Fermi's golden rule. Moreover Eq. (3.39) now manifests detailed balance, from which we immediately find that

$$\frac{f\left(\mathbf{p}+\hbar\mathbf{k}\right)}{f\left(\mathbf{p}\right)} = \frac{n_B\left(\frac{(\mathbf{p}+\hbar\mathbf{k})^2}{2m} - \frac{\mathbf{p}^2}{2m}\right)}{n_B\left(\frac{(\mathbf{p}+\hbar\mathbf{k})^2}{2m} - \frac{\mathbf{p}^2}{2m}\right) + 1} = \exp\left(-\beta\left(\frac{(\mathbf{p}+\hbar\mathbf{k})^2}{2m} - \frac{\mathbf{p}^2}{2m}\right)\right).$$

This implies that the only stationary reduced Wigner function for the system is given by a Maxwell-Boltzmann distribution. Note that this result is independent of the strength of the coupling γ and independent of the nature of the bath ω_k . With this in mind, we perturb the system by adding an external, uniform and stationary force, such that

$$H_0 = \frac{\mathbf{p}^2}{2m} - e\mathbf{E} \cdot \mathbf{x},$$

Since the bare system Hamiltonian remains quadratic we find

$$K_0\left(\mathbf{x},\mathbf{p},t|\mathbf{x}',\mathbf{p}',t'\right) = \delta\left(\mathbf{p} - \left(\mathbf{p}' + e\mathbf{E}\left(t - t'\right)\right)\right)\delta\left(\mathbf{x} - \left(\mathbf{x}' + \frac{\mathbf{p}'}{m}(t - t') + \frac{e\mathbf{E}}{2m}\left(t - t'\right)^2\right)\right).$$

If we again consider the initial distribution to be homogeneous, we arrive at the following Liouville equation for the perturbed system

$$\begin{pmatrix} \frac{\partial}{\partial t} + e\mathbf{E}\cdot\nabla_p \end{pmatrix} f(\mathbf{p},t) = \\ \sum_k \frac{2\left|\gamma(k)\right|^2}{\hbar^2} \int_0^\infty \mathrm{d}s \left[\begin{array}{c} n_B(\omega_k)\cos\left(E_+s/\hbar - \frac{\mathbf{k}\cdot e\mathbf{E}}{2m}s^2\right) \\ + \left(n_B(\omega_k) + 1\right)\cos\left(E_-s/\hbar - \frac{\mathbf{k}\cdot e\mathbf{E}}{2m}s^2\right) \end{array} \right] f\left(\mathbf{p} + \hbar\mathbf{k} - e\mathbf{E}s, t - s\right) \\ - \sum_k \frac{2\left|\gamma(k)\right|^2}{\hbar^2} \int_0^\infty \mathrm{d}s \left[\begin{array}{c} n_B(\omega_k)\cos\left(E_-s/\hbar - \frac{\mathbf{k}\cdot e\mathbf{E}}{2m}s^2\right) \\ + \left(n_B(\omega_k) + 1\right)\cos\left(E_+s/\hbar - \frac{\mathbf{k}\cdot e\mathbf{E}}{2m}s^2\right) \end{array} \right] f\left(\mathbf{p} - e\mathbf{E}s, t - s\right), \quad (3.40)$$

The right hand side of this equation is highly non-Markovian and difficult to treat. However, note that as a result of the bare propagator K_0 in the expression of the self-energy the Wigner function should be evaluated at a time s before the current time while also being displaced along the classical trajectory. In the absence of the bath, this would exactly yield the Wigner function at the current time. Hence under weak coupling conditions we have

$$f\left(\mathbf{p}-e\mathbf{E}s,t-s\right) \approx f\left(\mathbf{p},t\right) + \mathcal{O}\left(|\gamma(k)|^{2}\right),$$
$$f\left(\mathbf{p}+\hbar\mathbf{k}-e\mathbf{E}s,t-s\right) \approx f\left(\mathbf{p}+\hbar\mathbf{k},t\right) + \mathcal{O}\left(|\gamma(k)|^{2}\right).$$

As the right hand side of the equation of motion already contains a factor $|\gamma(k)|^2$ we can neglect the correction to the classical trajectory at weak coupling. This approximation results in the following Markovian Liouville equation

$$\left(\frac{\partial}{\partial t} + e\mathbf{E}\cdot\nabla_p\right) f\left(\mathbf{p}, t\right) \approx \sum_k \frac{2\pi |\gamma(k)|^2}{\hbar} \begin{bmatrix} n_B(\omega_k)S_+\left(\mathbf{p}, \mathbf{k}, \omega_k\right) \\ + \left(n_B(\omega_k) + 1\right)S_-\left(\mathbf{p}, \mathbf{k}, \omega_k\right) \end{bmatrix} f\left(\mathbf{p} + \hbar\mathbf{k}, t\right)$$
$$-\sum_k \frac{2\pi |\gamma(k)|^2}{\hbar} \begin{bmatrix} n_B(\omega_k)S_-\left(\mathbf{p}, \mathbf{k}, \omega_k\right) \\ + \left(n_B(\omega_k) + 1\right)S_+\left(\mathbf{p}, \mathbf{k}, \omega_k\right) \end{bmatrix} f\left(\mathbf{p}, t\right), \quad (3.41)$$

where

$$S_{\pm}(\mathbf{p}, \mathbf{k}, \omega_k) = \int_0^\infty \frac{\mathrm{d}\beta}{\pi} \cos\left(\beta E_{\pm} - \frac{\hbar^2 \mathbf{k} \cdot e\mathbf{E}}{2m}\beta^2\right).$$
(3.42)

Note that, although a single scattering event does not have to preserve energy anymore, the expected energy difference is still zero as the first moment of S_{\pm} with respect to E_{\pm} vanishes. It follows immediately that under linear response conditions, i.e., when the perturbation is weak, the scattering again becomes

$$\lim_{E \to 0} S_{\pm} \left(\mathbf{p}, \mathbf{k}, \omega_k \right) = \delta \left(\frac{\left(\mathbf{p} + \hbar \mathbf{k} \right)^2}{2m} - \frac{\mathbf{p}^2}{2m} \pm \hbar \omega_k \right),$$

and the reduced Liouville equation of the system simply becomes a classical linear Boltzmann equation where the scattering rates are given by Fermi's golden rule. Moreover note that the force dependent term in S_{\pm} is quantum in nature as it scales with \hbar^2 . In this respect the reduction of the scattering amplitudes to Fermi's golden rule under the assumption of vanishingly small perturbation can also be interpreted as a truncation of the exact quantum result up to the classical result, similar to the truncation of the Moyal bracket up to the classical Poisson bracket. Recall that this was the entire basis for the semiclassical perturbation theory for isolated systems presented in section 2.4. The β integral (3.42) which determines the scattering amplitude can, in this case, be done exactly as it is just a complex Gaussian integral. Doing so one finds that the resulting function tends to a delta function in a rather complicated way,



Figure 3.3: Scattering amplitude S_{\pm} for a system subjected to a constant external force. Here $\epsilon = \sqrt{\frac{2m}{|\mathbf{k} \cdot e\mathbf{E}|}} \frac{\Delta E_{\pm}}{\hbar} \operatorname{sgn}(\mathbf{k} \cdot e\mathbf{E})$.

as depicted in Fig. (3.3). Depending on the sign of $\mathbf{k} \cdot e\mathbf{E}$, the scattering amplitude oscillates rapidly or it decays monotonically. The oscillating behavior of the scattering amplitude again indicates the quantum nature of the scattering as it makes the scattering amplitude negative for some (non classical) transitions. In complete analogy with the previous chapter the correct quantum scattering probability should be considered a quasi probability as it can become negative. Once we truncate up to the classical result we again get a real probability, this time resulting in Fermi's golden rule. The scattering amplitude again illustrates the point made in the previous chapter. Although each term in the expansion of 3.42 has an additional component \hbar^2 we expand the function depicted in Fig. (3.3) in terms of increasingly singular functions. This is a very poor expansion of the scattering amplitude S_{\pm} itself. However one must always apply this scattering on a certain distribution. Whenever the distribution is wide enough, wider than the typical oscillations in S_{\pm} , all oscillations are washed out and the effect is more or less the same as scattering according to Fermi's golden rule. An expansion in terms of quantum corrections is thus possible in the high temperature limit. Analogous to the double slit experiment described in previous section, this is the limit in which almost no interference is present.

3.4.2 Low temperature linear response

Consider the bare Hamiltonian of the system to be

$$H_0 = \frac{\mathbf{p}^2}{2m} - e\mathbf{E}(t) \cdot \mathbf{x},$$

such that the bare propagator is

$$K_0(\mathbf{x}, \mathbf{p}, t | \mathbf{x}', \mathbf{p}', t') = \delta\left(\mathbf{p} - \mathbf{p}' - \int_{t'}^t e\mathbf{E}(s) \,\mathrm{d}s\right) \delta\left(\mathbf{x} - \mathbf{x}' - \frac{\mathbf{p}'}{m}(t - t') - \int_{t'}^t (t - \tau) \frac{e\mathbf{E}(\tau)}{m} \mathrm{d}\tau\right)$$
(3.43)

In contrast to the previous analyses we limit the present discussion to linear response, i.e. $|\mathbf{E}| \rightarrow 0$. The problem is still analytically intractable but we are only interested in finding the

conductivity (3.27). Knowledge of the (reduced) Wigner distribution function $f(\mathbf{p}, t)$ would allow to calculate the current density, and hence the conductivity σ

$$\mathbf{J}(t) = \frac{e}{m} \int \mathbf{p} f(\mathbf{p}, t) \, \mathrm{d}\mathbf{p} = \int_{-\infty}^{t} \sigma(t - t') \mathbf{E}(t') \mathrm{d}t'.$$
(3.44)

Instead of attempting to solve the full quantum Liouville equation we wish to derive an equation of motion for the current density itself. Multiplying the quantum Liouville equation with $e\mathbf{p}/m$ and integrating out the momentum yields

$$\int \frac{e\mathbf{p}}{m} \left(\frac{\partial}{\partial t} + e\mathbf{E}(t) \cdot \nabla_p \right) f(\mathbf{p}, t) \, \mathrm{d}\mathbf{p} = \int \mathrm{d}\mathbf{p}' \int_{-\infty}^t \mathrm{d}t' \sum_k \frac{2 |\gamma(k)|^2}{\hbar} \frac{e\mathbf{k}}{m} \times \\ \times \left\{ \begin{array}{c} n_B(\omega_k) \cos\left(\left[\mathbf{k} \cdot \left(\frac{\mathbf{p} + \hbar \mathbf{k}/2}{m} \right) - \omega_k \right] (t - t') + \int_{t'}^t (t - \tau) \frac{\mathbf{k} \cdot e\mathbf{E}(s)}{m} \mathrm{d}\tau \right) \\ + (n_B(\omega_k) + 1) \cos\left(\left[\mathbf{k} \cdot \left(\frac{\mathbf{p}' + \hbar \mathbf{k}/2}{m} \right) + \omega_k \right] (t - t') + \int_{t'}^t (t - \tau) \frac{\mathbf{k} \cdot e\mathbf{E}(s)}{m} \mathrm{d}\tau \right) \end{array} \right\} f(\mathbf{p}', t') \,,$$

where the self energy (3.37) is calculated with the driven particle propagator (3.43). Taking the expression (3.44) for the current density into account, the left hand side can directly be calculated. Furthermore using $\mathbf{k} \leftrightarrow -\mathbf{k}$ symmetry of the right hand side, the expression results in

$$\frac{d\mathbf{J}(t)}{dt} - \frac{n_0 e^2}{m} \mathbf{E}(t) = -\int_{-\infty}^t \mathrm{d}s \sum_k \frac{2 |\gamma(k)|^2}{\hbar} \frac{\mathbf{k}}{m} \begin{bmatrix} n_B(\omega_k) \sin\left(\left(\frac{\hbar k^2}{2m} - \omega_k\right)(t-s)\right) \\ + (n_B(\omega_k) + 1) \sin\left(\left(\frac{\hbar k^2}{2m} + \omega_k\right)(t-s)\right) \end{bmatrix} \times e \int \mathrm{d}\mathbf{p} \sin\left(\frac{\mathbf{k} \cdot \mathbf{p}}{m} (t-s) + \int_s^t (t-\tau) \frac{\mathbf{k} \cdot e \mathbf{E}(\tau)}{m} \mathrm{d}\tau\right) f(\mathbf{p}, s). \quad (3.45)$$

Since the current density (3.44) is of order **E**, the dominant contribution in the last line of this equation is provided by the small momenta. It thus seems reasonable to expand the sine function. For general coupling strength $\gamma(k)$ and temperature, this expansion seems not very useful. Indeed, the Wigner function broadens with increasing temperature. Furthermore, for strong coupling the initial phonon states are better described by displaced and broadened Gaussian wave functions, as shown in the derivation of the optical absorption of polarons in [43, 44].

Therefore, for $\gamma(k)$ and T sufficiently small, one might truncate the expansion to the first moment, which results in

$$\frac{d\mathbf{J}(t)}{dt} - \frac{n_0 e^2}{m} \mathbf{E}(t) \approx -\int_{-\infty}^t \mathrm{d}s \sum_k \frac{2 |\gamma(k)|^2}{\hbar} \frac{\mathbf{k}}{m} \begin{bmatrix} n_B(\omega_k) \sin\left(\left(\frac{\hbar k^2}{2m} - \omega_k\right)(t-s)\right) \\ + (n_B(\omega_k) + 1) \sin\left(\left(\frac{\hbar k^2}{2m} + \omega_k\right)(t-s)\right) \end{bmatrix} \times \\ \times \left(\frac{\mathbf{k} \cdot \mathbf{J}(s)}{m} (t-s) + \frac{n_0 e^2}{m} \int_s^t (t-\tau) \frac{\mathbf{k} \cdot \mathbf{E}(\tau)}{m} \mathrm{d}\tau \right) \quad (3.46)$$

Since the coupling is isotropic the latter finally results in the following expression for the current density

$$\frac{d\mathbf{J}(t)}{dt} + \int_{-\infty}^{t} \mathbf{J}(s)\chi(t-s)ds = \frac{n_0 e^2}{m}\mathbf{E}(t) - \frac{n_0 e^2}{m}\int_{-\infty}^{t}\kappa(t-s)\mathbf{E}(s)ds, \qquad (3.47)$$

where the memory function χ of the system is given by

$$\chi(t) = t \sum_{\mathbf{k}} \frac{2 |\gamma(k)|^2}{3\hbar} \frac{\mathbf{k}^2}{m} \left\{ \begin{array}{c} \left(n_B\left(\omega_k\right) + 1 \right) \sin\left(\left[\frac{\hbar \mathbf{k}^2}{2m} + \omega_k \right] t \right) \\ + n_B\left(\omega_k\right) \sin\left(\left[\frac{\hbar \mathbf{k}^2}{2m} - \omega_k \right] t \right) \end{array} \right\},$$
(3.48)

and the polarizability κ becomes

$$\kappa(t) = t \int_{t}^{\infty} d\tau \sum_{k} \frac{2 |\gamma(\mathbf{k})|^{2}}{3\hbar} \frac{\mathbf{k}^{2}}{m} \left\{ \begin{array}{c} n_{B}(\omega_{k}) \sin\left(\left\lfloor \frac{\hbar \mathbf{k}^{2}}{2m} - \omega_{k} \right\rfloor \tau\right) \\ + (n_{B}(\omega_{k}) + 1) \sin\left(\left\lfloor \frac{\hbar \mathbf{k}^{2}}{2m} + \omega_{k} \right\rfloor \tau\right) \end{array} \right\}$$
$$= t \int_{t}^{\infty} d\tau \frac{\chi(\tau)}{\tau}.$$
(3.49)

The definition (3.27) of the conductivity thus yields the following relation between the Laplace transform $\mathcal{L}(\sigma, \Omega)$ of the conductivity and the Laplace transform $\mathcal{L}(\chi, \Omega)$ and $\mathcal{L}(\kappa, \Omega)$ of the memory function and polarizability respectively:

$$\mathcal{L}(\sigma, \Omega) = \frac{n_0 e^2}{m} \frac{1 - \mathcal{L}(\kappa, \Omega)}{\Omega + \mathcal{L}(\chi, \Omega)}.$$

A more accurate conductivity can be found using a resummation argument similar to that in the previous section. The bare propagator K_0 and the true propagator K are identical up to $\mathcal{O}\left(|\gamma(k)|^2\right)$. Consequently the true polarizability depends on the conductivity of the system. Taking this feedback into account approximately yields

$$\mathcal{L}(\sigma,\Omega) = \frac{n_0 e^2}{m} \frac{1}{\Omega + (\Omega \mathcal{L}(\kappa,\Omega) + \mathcal{L}(\chi,\Omega))}.$$
(3.50)

Of course at very small coupling the resummation would not matter. Note that this expression is structurally similar to (3.28), which was obtained from a linear Caldeira-Leggett type of model, i.e. we should compare $\mathcal{L}(\chi, \Omega)$ with $(m\Omega)^{-1}\mathcal{L}(A, \Omega)$. Both expressions actually have the prefactor $|\gamma(k)|^2 \mathbf{k}^2$ and the division of $A(\Omega)$ by Ω has changed into a multiplication by t in $\chi(t)$. To obtain the Caldeira-Leggett result, the coupling was linearized in \mathbf{k} . Such a linearization is poorly controlled as it is already done on the level of the Hamiltonian and it does not take into account the state of the system. The present approach however linearizes in \mathbf{p} . This is profoundly different. The goodness of the linearization in \mathbf{p} is controlled by the shape of the distribution function. We found that in order for the approximation to be valid both the coupling and the temperature need to be sufficiently small. The real difference between the two is actually the dependence on temperature and the appearance of the recoil energy $(\hbar \mathbf{k})^2 / 2m$ of the jump in the memory function $\chi(t)$. This is absent in the previous linear model because it linearized in the size of the jump k. In the next section we compare the results for the Fröhlich polaron.

3.4.3 The Fröhlich polaron

For the optical Fröhlich polaron one considers $\omega_k = \omega_{LO} = 1$ to be constant. In this section we set $\hbar = m = 1$. The coupling

$$\left|\gamma\left(k\right)\right|^{2} = \frac{1}{k^{2}} \frac{2\sqrt{2\pi\alpha}}{V} \tag{3.51}$$

scales with the dimensionless coupling constant α . Then, in the continuum limit, the remaining integral in Eq. (3.48) is Gaussian and results in

$$\chi(t) = \frac{\sqrt{2\alpha}}{3\sqrt{\pi}} \left[(2n_B + 1) \frac{\cos(t)}{\sqrt{t}} - \frac{\sin(t)}{\sqrt{t}} \right] = \frac{\alpha}{3} \left[(2n_B + 1) J_{-1/2}(t) - J_{1/2}(t) \right],$$

where $J_{\pm 1/2}$ denotes the Bessel function of the first kind of order $\pm 1/2$. The Laplace transform [45] of χ is given by

$$\mathcal{L}(\chi,\Omega) = \frac{\alpha}{3\sqrt{\Omega^2 + 1}} \left((2n_B + 1)\sqrt{\sqrt{\Omega^2 + 1} + \Omega} - \sqrt{\sqrt{\Omega^2 + 1} - \Omega} \right).$$
(3.52)



Figure 3.4: Optical absorption coefficient for Fröhlich polaron at T = 0 for $\alpha = 0.01$. The full blue line represent the present result and the red circles (DHL) are a perturbative result by Devreese *et al.* [46].

The T = 0 Laplace transformed polarizability $\mathcal{L}(\kappa, \Omega)$ is given by the following integral

$$\mathcal{L}(\kappa,\Omega) = \frac{4\alpha}{3\pi} \int_{-\infty}^{\infty} du \ u^2 \frac{\Omega^2 - (u^2 + 1)^2}{(u^2 + 1)\left((u^2 + 1)^2 + \Omega^2\right)^2}$$

which can readily be done by using Cauchy's residue theorem, which yields

$$\mathcal{L}(\kappa,\Omega) = \frac{\sqrt{2}\alpha}{3\Omega^2} \frac{\Omega^2 + 2 + 2\sqrt{\Omega^2 + 1}\left(1 - \sqrt{2}\sqrt{\sqrt{\Omega^2 + 1} + 1}\right)}{\sqrt{\Omega^2 + 1}\sqrt{\sqrt{\Omega^2 + 1} + 1}}$$

The zero temperature optical absorption is depicted in Fig. (3.4) and Fig. (3.5) for $\alpha = 0.01$ and $\alpha = 1$ respectively. As anticipated, the behavior is drastically different from the one predicted by the linearized Caldeira-Leggett model (3.28) depicted in Fig. (3.1). For comparison Fig. (3.4) also shows a weak coupling result due to Devreese *et al.* [46] (hereafter referred to as DHL). Their result is perturbative in α and thus becomes exact for $\alpha \to 0$. For $\alpha = 0.01$ their result is indistinguishable from the present result, which implies the present truncation scheme correctly predicts the weak coupling optical absoprtion. For $\alpha = 1$ we show the absorption spectrum in Fig. (3.5). At this point there is a clear distinction between the present approach and the DHL result. We therefore compare the result with the absorption obtained from a diagrammatic quantum Monte Carlo calculation [47], which should give numerically exact answers for all α . Although the present result is distinguishable from the Monte Carlo calculation, it is clearly more accurate than the perturbative result of DHL. Moreover, the present result is remarkably close to the nonperturbative method presented in Ref. [38]. The method, due to Devreese et al. [38], employs the impedance function approximation of FHIP [42]. The method is thus nonperturbative in the sense that no expansion in the coupling constant is assumed. Although the zero temperature optical absorption based on the FHIP approximation agrees well with the exact numerical results for weak to intermediate coupling constants [48], the FHIP approximation predicts an incorrect temperature dependence of the weak coupling low temperature polaron mobility.



Figure 3.5: Optical absorption coefficient for Fröhlich polaron at T = 0 for $\alpha = 1$. The full blue line represent the present result, the dashed red line (DHL) is a perturbative result by Devreese *et al.* [46]. Furthermore, the dashed green line (DSG) is a variational result due to Devreese *et al.* [38] and the circles (DQMC) show a numerical result due to Mishchenko *et al.* [47,48].DSG and DQMC data copied with permission of the authors from [49]

Note that in contrast to the Caldeira-Leggett model the present result has a central peak with a height and a width controlled by the temperature. Consequently we can study the low temperature dc-conductivity

$$\sigma_{dc} = \lim_{\Omega \to 0} \mathcal{L}\left(\sigma, \Omega\right) = \frac{3e^2 n_0}{2\alpha n_B} \approx \frac{3e^2 n_0}{2\alpha} e^{\beta}.$$
(3.53)

It should immediately be noted that this result differs by a factor of 3 from that of Kadanoff [41] and by a factor of (2β) from that of FHIP [42], i.e.,

$$\sigma_{dc} = \mathop{3}_{\text{Kadanoff}} \sigma_{dc} = 2\beta \sigma_{dc} \,. \tag{3.54}$$

The result is in agreement with a prediction by Los' [50] based on a Green's superoperator calculation of Kubo's formula. It was already argued by FHIP, that in the $\Omega \to 0$ limit the full Boltzmann equation should be solved in order to get an accurate result for the dc mobility, an approximate solution of which was later provided by Kadanoff [41]. It was furthermore argued, in Ref. [51,52], that the 3/(2 β) discrepancy was caused by an interchange of the $\Omega \to 0$ and $\alpha \to 0$ limit. One might wonder whether interchanging similar limits gives different results in the current approach. The equation of motion for the current density was obtained by expanding the scattering term around $p \to 0$. One might guess that interchanging the limits by first taking the limit of $\Omega \to 0$, hence $t \to \infty$, and then the limit of $p \to 0$ will result in a similar difference. As argued in detail in appendix C.1 this is not the case.

The discussion in appendix C.1 furthermore immediately explains the factor of 3 discrepancy between the present model and the result of Kadanoff. The in-scattering term in the Boltzmann equation, expressed in terms of the angular correlation factor in [41], is completely neglected by Kadanoff and dismissed as vanishingly small. But neglecting this in-scattering violates particle number conservation. Within the present approach the in-scattering component is nonvanishing. The component linear in E exactly subtracts $2/3(2\alpha)$ from the inverse scattering rate resulting in a mobility which is three times higher than the one calculated within the relaxation time approximation. It is clear that the present approach does not violate particle number conservation, neither does FHIP nor Los'. It should be noted that this explanation is in agreement with the one presented in [50] by Los'.

The additional 2β difference with FHIP however remains to be explained. In appendix C.2 we reexamine the FHIP approximation in the language of the distribution function rather than path integrals for the reduced density matrix. This illuminates the main problem in the FHIP approximation. First and foremost, unlike what is argued by FHIP, it is detrimental to assume an initial product state between the bath and the system for the evolution of the model. Although the true system will quickly thermalize to the temperature of the bath, the model system of FHIP does not thermalize, because it is completely harmonic. In order to obtain a physical trial distribution one must assume that the complete model system was in thermal equilibrium instead of in a product state of the system with a thermal bath. Apart from this small change the analysis in appendix C.2 is completely in line with FHIP. The final low temperature dc-conductivity however reads

$$\sigma_{dc} = \frac{3e^2n_0}{2\alpha m^*}e^\beta.$$

where the effective mass $m^*/m = v^2/w^2$ is defined in terms of Feynman's variational parameters. Since $w \approx v$ and thus $m^* \approx m$ for sufficiently small α , we recover the same result (3.53) as derived by our linearized equation of motion. It is clear that the present FHIP reanalysis does not have the spurious 2β terms. In conclusion we find that, whereas the relaxation time approximation used by Kadanoff explicitly violates particle number conservation, the method developed by FHIP does not. The FHIP approximation however relies on an unphysical initial state for Feynman's polaron model. A slightly modified version of both, which amends these two problems, accounts for their discrepancy.

3.4.4 Mobility, effective mass and dynamical screening

Let us focus on the problem of extracting the dc-conductivity and the effective mass from the previous results. If we have the Laplace transformed memory function $\mathcal{L}(\chi, \Omega)$ and polarizability $\mathcal{L}(\kappa, \Omega)$, we can of course extract the dc-conductivity in the manner we have discussed in the previous section. It is however clear that both the mobility and the effective mass only require knowledge of these functions near $\Omega = 0$. Consider the expansions

$$\mathcal{L}(\chi, \Omega) = \chi_0 + \chi_1 \Omega + O(\Omega^2),$$

$$\mathcal{L}(\kappa, \Omega) = \kappa_0 + \kappa_1 \Omega + O(\Omega^2).$$

Then we find the low energy optical absorption

$$\operatorname{Re}\left[\mathcal{L}\left(\sigma,i\omega\right)\right] \approx \frac{e^{2}\pi}{m\left(1+\chi_{1}+\kappa_{0}\right)}\left[\frac{1}{\pi}\frac{\gamma}{\omega^{2}+\gamma^{2}}\right],$$

where $\gamma = \chi_0 (1 + \chi_1 + \kappa_0)^{-1}$. Note that the term between brackets is a Lorentzian distribution with a width γ . Consequently when $\gamma = 0$, it results in a delta function $\delta(\omega)$. From this we readily identify the effective mass

$$\frac{m^*}{m} = (1 + \chi_1 + \kappa_0) = 1 + \frac{\chi_1}{2}.$$
(3.55)

The latter equality immediately follows from the definition (3.49) of $\kappa(t)$ in terms of $\chi(t)$. For finite χ_0 , the dc-conductivity is finite and given by

$$\sigma_{dc} = \frac{n_0 e^2}{m\chi_0}.$$



Figure 3.6: Optical absorption coefficient for Fröhlich polaron at T = 0 for $\alpha = 1$. The full blue line represent the present result and the red dashed line represent the result without dynamical screening, i.e. $\kappa(t) = 0$.

Consequently, for every finite κ_0 the dc-conductivity is equal to the dc-conductivity of the system without dynamical screening, i.e. $\kappa(t) = 0$. For stationary properties the effect of dynamical screening is thus of second order. In contrast to the mobility the effective mass of the system is significantly altered by dynamical screening. In fact the relative change in the mass is only half of the change without dynamical screening. It should be noted that effective mass is a dynamical quantity and it depends on the entire spectral function through the polaron-f-sum rule [53] by Devreese *et al.*. Consequently, a redistribution of spectral weight must accompany the change in effective mass. This is illustrated for the Fröhlich polaron in Fig. (3.6).

The coefficients $\chi_{0,1}$ can be found by expanding the expression for the Laplace transform of χ . Consequently

$$\chi_0 = \int_0^\infty \chi(t) dt$$
, and $\chi_1 = -\int_0^\infty t \chi(t) dt$.

are the two lowest moments of the real time memory function. Plugging in the continuum limit of expression (3.48) we arrive at

$$\begin{split} \chi_{0} &= -\int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^{d}} \frac{2\pi V \left|\gamma\left(k\right)\right|^{2}}{3\hbar} \frac{\mathbf{k}^{2}}{m} \left[\left(n_{B}\left(\omega_{k}\right)+1\right) \delta'\left(\frac{\hbar \mathbf{k}^{2}}{2m}+\omega_{k}\right)+n_{B}\left(\omega_{k}\right) \delta'\left(\frac{\hbar \mathbf{k}^{2}}{2m}-\omega_{k}\right) \right],\\ \chi_{1} &= \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^{d}} \frac{4V \left|\gamma\left(k\right)\right|^{2}}{3\hbar} \frac{\mathbf{k}^{2}}{m} \left[\frac{n_{B}\left(\omega_{k}\right)+1}{\left(\frac{\hbar \mathbf{k}^{2}}{2m}+\omega_{k}\right)^{3}}+\frac{n_{B}\left(\omega_{k}\right)}{\left(\frac{\hbar \mathbf{k}^{2}}{2m}-\omega_{k}\right)^{3}} \right],\end{split}$$

where d is the dimensionality of the problem, V is the volume and $\delta'(x)$ is the derivative of a Dirac delta function. Again the expression for χ_0 ought to be compared with the expression for the inverse scattering time (C.3) within the relaxation time approximation. For the 3D Fröhlich polaron we obtain

$$\chi_{0} = rac{2lpha\omega_{LO}n_{B}\left(\omega_{LO}
ight)}{3}, ext{ and } \chi_{1} = rac{lpha}{3}\left(1 + n_{B}\left(\omega_{LO}
ight)
ight),$$

which indeed yields the conductivity (3.53). The present truncation scheme moreover predicts a zero temperature effective mass of $m^*/m = (1 + \alpha/6)$, in agreement with standard weak coupling theories. For an excellent in-depth overview and discussion on this topic we refer to a textbook by Alexandrov and Devreese [54] and to lecture notes by Devreese [55].

Chapter 4

Quantum field theory

This chapter is concerned with a second quantized description of the Wigner distribution and its propagation in time. We thus generalize the results presented in chapter 2. The discussion is limited to bosonic field theories. After generalizing the Wigner distribution and its propagator to a quasi distribution and quasi conditional probability of fields, we again discuss semiclassical approximation methods in section (4.2.2). One can approach this generalization in different ways. A prominent approach, due to Polkovnikov, can be found in [7]. Here we adopt a slightly different point of view, one that does not explicitly involve coherent states. Although the result is the same I believe the present approach is more pedagogical and at the same time more flexible.

4.1 Phase space propagator of fields

Previous section focused on a particle interacting with a set of harmonic oscillators, the generic polaron problem. The harmonic oscillators model various bosonic fields such as phonons, photons, Bogoliubov excitations, *etc.*. In the previous section we started from a second quantized description of the fields in terms of creation and annihilation operators and used Dirac ladder operators to cast them into a set of harmonic oscillators. Here we are concerned with the opposite problem. We will keep the description in terms of creation and annihilation operators and annihilation operators and transform our phase space instead.

Consider the definition (2.15) of the propagator for a single particle system, which I repeat here for convenience

$$f(x_b, p_b, t_b) = \iint K_w(x_b, p_b, t_b | x_a, p_a, t_a) f(x_a, p_a, t_a) dx_a dp_a, \qquad (4.1)$$

and the propagator (2.24) in terms of the Hamiltonian of the system

$$K_w(x_b, p_b, t_b | x_a, p_a, t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \int_{p(t_a)=p_a}^{p(t_b)=p_b} \mathcal{D}p \iint \frac{\mathcal{D}\xi \mathcal{D}\kappa}{(2\pi\hbar)^2} \exp\left\{-\frac{i}{\hbar} \int_{t_a}^{t_b} \left[\dot{p}\xi - \dot{x}\kappa + H\left(x + \frac{\xi}{2}, p + \frac{\kappa}{2}\right) - H\left(x - \frac{\xi}{2}, p - \frac{\kappa}{2}\right)\right] \mathrm{d}t\right\}.$$

The single particle phase space is spanned by the generalized coordinate and its conjugate momentum. These are just two numbers and it is tempting, albeit with hindsight, to consider

instead a single complex number ψ as the phase space variable,

$$x = \sqrt{\frac{2\hbar}{m\omega}} \operatorname{Re}(\psi) = \sqrt{\frac{\hbar}{2m\omega}} \left(\bar{\psi} + \psi\right),$$
$$p = \sqrt{2\hbar m\omega} \operatorname{Im}(\psi) = i\sqrt{\frac{\hbar m\omega}{2}} \left(\bar{\psi} - \psi\right),$$

such that considering the propagator to move between two phase space points (x_a, p_a) and (x_b, p_b) , becomes identical to the conditional quasi probability to move from ψ_a to ψ_b . Here $\bar{\psi}$ denotes the complex conjugate of ψ . Let us also define

$$\xi = \sqrt{\frac{2\hbar}{m\omega}} \operatorname{Re}(\chi),$$

$$\kappa = \sqrt{2\hbar m\omega} \operatorname{Im}(\chi),$$

and simply substitute these expression into the general expression for the propagator

$$K_{w}\left(\psi_{b},\bar{\psi}_{b},t_{b}|\psi_{a},\bar{\psi}_{a},t_{a}\right) = \int_{\psi(t_{a})=\psi_{a}}^{\psi(t_{b})=\psi_{b}} \mathcal{D}\psi \mathcal{D}\bar{\psi} \int \int \mathcal{D}\chi \mathcal{D}\bar{\chi} \exp\left(-\frac{i}{\hbar}\int_{t_{a}}^{t_{b}}\left(i\hbar\partial_{t}\bar{\psi}\chi-i\hbar\partial_{t}\psi\bar{\chi}\right)\mathrm{d}t\right) \\ \times \exp\left\{-\frac{i}{\hbar}\int_{t_{a}}^{t_{b}}\left[H\left(\psi+\frac{\chi}{2},\bar{\psi}+\frac{\bar{\chi}}{2}\right)-H\left(\psi-\frac{\chi}{2},\bar{\psi}-\frac{\bar{\chi}}{2}\right)\right]\mathrm{d}t\right\},$$

where by definition

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$$\iint \mathcal{D}\chi \mathcal{D}\bar{\chi} \equiv \iint \frac{\mathcal{D}\operatorname{Re}(\chi) \mathcal{D}\operatorname{Im}(\chi)}{\pi}, \qquad (4.2)$$

$$\iint_{\psi(t_a)=\psi_a} \mathcal{D}\psi \mathcal{D}\bar{\psi} \equiv \int_{\operatorname{Re}[\psi(t_a)]=\operatorname{Re}[\psi_a]}^{\operatorname{Re}[\psi(t_b)]=\operatorname{Re}[\psi_b]} \int_{\operatorname{Im}[\psi(t_a)]=\operatorname{Im}[\psi_a]}^{\operatorname{Im}[\psi(t_b)]=\operatorname{Im}[\psi_b]} \frac{\mathcal{D}\operatorname{Re}(\psi)\mathcal{D}\operatorname{Im}(\psi)}{\pi}, \quad (4.3)$$

$$H(\psi, \bar{\psi}) \equiv H\left(\sqrt{\frac{2\hbar}{m\omega}} \operatorname{Re}[\psi], \sqrt{2\hbar m\omega} \operatorname{Im}[\psi]\right).$$
(4.4)

At this point we have already obtained the single mode result and it can readily be generalized to the many mode case by defining

$$\psi^{T} \equiv (\psi_{1}, \psi_{2}, ..., \psi_{N})$$
$$\mathrm{d}\psi \mathrm{d}\bar{\psi} \equiv \prod_{i=1}^{N} \mathrm{d}\psi_{i} \mathrm{d}\bar{\psi}_{i}.$$

Then we find

$$f\left(\boldsymbol{\psi}_{b}, \bar{\boldsymbol{\psi}}_{b}, t_{b}\right) = \iint K_{w}\left(\boldsymbol{\psi}_{b}, \bar{\boldsymbol{\psi}}_{b}, t_{b} | \boldsymbol{\psi}_{a}, \bar{\boldsymbol{\psi}}_{a}, t_{a}\right) f\left(\boldsymbol{\psi}_{a}, \bar{\boldsymbol{\psi}}_{a}, t_{a}\right) \mathrm{d}\boldsymbol{\psi}_{a} \mathrm{d}\bar{\boldsymbol{\psi}}_{a}, \tag{4.5}$$

where the propagator is given by

and ψ^{\dagger} is the Hermitian conjugate of ψ , i.e. $\psi^{\dagger} = \bar{\psi}^{T}$. This expression for the propagator generalizes expression (2.24). Here we have presented a rather formal derivation using the standard canonical quantization techniques. The same result can however be obtained by using the generality of Feynman's Lagrangian description of quantum mechanics. Any action can be used to compute the amplitude and one could thus simply start from a Lagrangian density for a field theory rather than a Lagrangian for a point particle. One could argue that in that case the Wigner-Weyl transformation is not immediately defined, but in analogy with the derivation for the corpuscular particle one would actually like the transformation to absorb the boundary terms obtained from the integration by parts. This is required in order to get an unconstrained path integral for the auxiliary field. This yields the following definition for the Wigner function

$$f(\boldsymbol{\psi}, \boldsymbol{\bar{\psi}}) = \int \left\langle \boldsymbol{\psi} + \frac{\boldsymbol{\chi}}{2} \right| \hat{\rho} \left| \boldsymbol{\psi} - \frac{\boldsymbol{\chi}}{2} \right\rangle \exp\left(\frac{1}{2} \left(\boldsymbol{\psi}^{\dagger} \boldsymbol{\chi} - \boldsymbol{\chi}^{\dagger} \boldsymbol{\psi}\right)\right) \frac{\mathrm{d}\boldsymbol{\chi} \mathrm{d}\boldsymbol{\bar{\chi}}}{2^{N}}, \tag{4.7}$$

where N is again the size of the Hilbert space. Moreover, for the analogy to be complete, $|\psi\rangle$ should be the eigenstate of $\hat{\psi}$, i.e. $\hat{\psi} |\psi\rangle = \psi |\psi\rangle$ such that $|\psi\rangle$ is a coherent state. This derivation reproduces the rigorous definition [7] of the Wigner function, it is moreover a more flexible approach and I believe such flexibility holds the key to generalizing the propagator to fermionic fields.

4.1.1 Non-interacting theories

Consider any time dependent harmonic Hamiltonian

$$H\left(oldsymbol{\psi},ar{oldsymbol{\psi}}
ight)=oldsymbol{\psi}^{\dagger}\mathbf{H}oldsymbol{\psi}_{2}$$

where **H** is an $N \times N$ matrix, then

$$H\left(\psi+\frac{\chi}{2}, \bar{\psi}+\frac{\bar{\chi}}{2}\right) - H\left(\psi-\frac{\chi}{2}, \bar{\psi}-\frac{\bar{\chi}}{2}\right) = \chi^{\dagger}\mathbf{H}\psi + \psi^{\dagger}\mathbf{H}\chi.$$

In this case the propagator can be explicitly evaluated:

$$K_{w} = \int_{\psi(t_{a})=\psi_{a}}^{\psi(t_{b})=\psi_{b}} \mathcal{D}\psi \mathcal{D}\bar{\psi} \int \int \mathcal{D}\chi \mathcal{D}\bar{\chi} \exp\left\{-\frac{i}{\hbar} \int_{t_{a}}^{t_{b}} \left(\begin{array}{c} \left[i\hbar\partial_{t}\psi^{\dagger}\mathbf{I}+\psi^{\dagger}\mathbf{H}\right]\chi\\-\chi^{\dagger}\left[\mathbf{I}i\hbar\partial_{t}\psi^{\dagger}-\mathbf{H}\psi\right]\end{array}\right) \mathrm{d}t\right\}$$
$$= \int_{\psi(t_{a})=\psi_{a}}^{\psi(t_{b})=\psi_{b}} \mathcal{D}\psi \mathcal{D}\bar{\psi}\delta\left[i\hbar\partial_{t}\bar{\psi}+\mathbf{H}\bar{\psi}\right]\delta\left[i\hbar\partial_{t}\psi-\mathbf{H}\psi\right].$$

Consequently, in complete agreement with the result in first quantization, we find that of all possible paths only the classical trajectory contributes to the path integral except that in this case the classical limit yields the Schrödinger equation for the fields rather than Newtonian equations of motion for the point particle. For non-harmonic, interacting, problems the problem is in general not analytically solvable. We thus need to consider generalizations of the approximations presented in chapter 2. It is clear that all results are immediately transferable since we have only enlarged our Hilbert space and relabeled our phase space variables. In order to provide a different perspective to the discussion in chapter 2, we will adopt a generating function approach here. Instead of doing this in the most general setting let us do this for massive bosons interacting trough s-wave scattering, a common situation in cold atom systems.

4.2 s-wave interacting Bosons

Consider a bosonic field with the following (Weyl-ordered) Hamiltonian

$$H = \int \left(\frac{\hbar^2}{2m} \nabla \bar{\psi}(x) \cdot \nabla \psi(x) + \bar{\psi}(x) V(x) \psi(x)\right) dx + \frac{1}{2} \iint \bar{\psi}(x) \bar{\psi}(x') V_{\text{int}}(x - x') \psi(x') \psi(x) dx dx'.$$
(4.8)

Furthermore, consider an interaction potential

 $V_{\text{int}}(x) = g\delta(x).$

Then the continuum limit of propagator (4.6) becomes

$$K_{w}\left(\boldsymbol{\psi}_{b}, \bar{\boldsymbol{\psi}}_{b}, t_{b} | \boldsymbol{\psi}_{a}, \bar{\boldsymbol{\psi}}_{a}, t_{a}\right) = \int_{\psi(t_{a})=\psi_{a}}^{\psi(t_{b})=\psi_{b}} \mathcal{D}\boldsymbol{\psi}\mathcal{D}\bar{\boldsymbol{\psi}} \int \mathcal{D}\boldsymbol{\chi}\mathcal{D}\bar{\boldsymbol{\chi}}$$

$$\exp\left\{\frac{i}{\hbar} \int \int \left[-i\hbar \frac{\partial \bar{\psi}(x)}{\partial t} + \frac{\hbar^{2}}{2m} \nabla^{2} \bar{\psi}(x) - \left(g |\psi(x)|^{2} + V(x)\right) \bar{\psi}(x)\right] \chi(x) dx dt + \frac{i}{\hbar} \int \int \left[i\hbar \frac{\partial \psi(x)}{\partial t} + \frac{\hbar^{2}}{2m} \nabla^{2} \psi(x) - \left(g |\psi(x)|^{2} + V(x)\right) \psi(x)\right] \bar{\chi}(x) dx dt + \frac{i}{\hbar} \int \int \left[i\hbar \frac{\partial \psi(x)}{\partial t} + \frac{\hbar^{2}}{2m} \nabla^{2} \psi(x) - \left(g |\psi(x)|^{2} + V(x)\right) \psi(x)\right] \bar{\chi}(x) dx dt + \frac{i}{\hbar} \int \int \left[i\hbar \frac{\partial \psi(x)}{\partial t} + \frac{\hbar^{2}}{2m} \nabla^{2} \psi(x) - \left(g |\psi(x)|^{2} + V(x)\right) \psi(x)\right] \bar{\chi}(x) dx dt + \frac{i}{\hbar} \int \int \left[i\hbar \frac{\partial \psi(x)}{\partial t} + \frac{\hbar^{2}}{2m} \nabla^{2} \psi(x) - \left(g |\psi(x)|^{2} + V(x)\right) \psi(x)\right] \bar{\chi}(x) dx dt + \frac{i}{\hbar} \int \int \left[i\hbar \frac{\partial \psi(x)}{\partial t} + \frac{\hbar^{2}}{2m} \nabla^{2} \psi(x) - \left(g |\psi(x)|^{2} + V(x)\right) \psi(x)\right] \bar{\chi}(x) dx dt + \frac{i}{\hbar} \int \int \left[i\hbar \frac{\partial \psi(x)}{\partial t} + \frac{\hbar^{2}}{2m} \nabla^{2} \psi(x) - \left(g |\psi(x)|^{2} + V(x)\right) \psi(x)\right] \bar{\chi}(x) dx dt + \frac{i}{\hbar} \int \int \left[i\hbar \frac{\partial \psi(x)}{\partial t} + \frac{\hbar^{2}}{2m} \nabla^{2} \psi(x) - \left(g |\psi(x)|^{2} + V(x)\right) \psi(x)\right] \bar{\chi}(x) dx dt + \frac{i}{\hbar} \int \int \left[i\hbar \frac{\partial \psi(x)}{\partial t} + \frac{\hbar^{2}}{2m} \nabla^{2} \psi(x) - \left(g |\psi(x)|^{2} + V(x)\right) \psi(x)\right] dx dt \right\}.$$

$$(4.9)$$

It is clear that this path integral can not be solved by standard techniques because of the $O(\chi^3)$ in the last line. By expanding the last line in a series around $\chi = 0$ we again generate the perturbation series around the classical result, as derived for point particles in chapter 2. Here we adopt a different approach to provide an alternative perspective on the exponential complexity of the problem. It moreover provides additional insight in other stochastic or collective auxiliary field methods, in particular the Hubbard-Stratanovich [57,58] transformation. In the context of non-equilibrium quantum dynamics, similar work on the stochastic representation of quantum field theories was performed by L. Plimak, M. Olsen and collaborators [6, 59, 60].

4.2.1 Noisy Gross-Pitaevskii trajectories

One can separate the linear terms in χ from the cubic terms by introducing an additional auxiliary field $\eta(x)$, i.e. define

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + \left(g\left|\psi\right|^2 + V\right)\psi + \eta, \qquad (4.10)$$

$$-i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\bar{\psi} + \left(g\left|\psi\right|^2 + V\right)\bar{\psi} + \bar{\eta}.$$
(4.11)

Note that we have dropped the explicit dependence of the fields on space-time in order not to overload the notation. Using this definition we can rewrite the propagator as

$$K_{w}\left(\boldsymbol{\psi}_{b}, \bar{\boldsymbol{\psi}}_{b}, t_{b} | \boldsymbol{\psi}_{a}, \bar{\boldsymbol{\psi}}_{a}, t_{a}\right) = \int_{\psi(t_{a})=\psi_{a}}^{\psi(t_{b})=\psi_{b}} \mathcal{D}\boldsymbol{\psi}\mathcal{D}\bar{\boldsymbol{\psi}} \int \int \mathcal{D}\boldsymbol{\chi}\mathcal{D}\bar{\boldsymbol{\chi}} \int \int \mathcal{D}\boldsymbol{\eta}\mathcal{D}\bar{\boldsymbol{\eta}}\delta\left[(4.10)\right]\delta\left[(4.11)\right] \\ \exp\left\{\frac{i}{\hbar} \int \int \left[(\bar{\eta}\chi + \eta\bar{\chi}) - \frac{g}{4} |\chi|^{2} \left(\psi\bar{\chi} + \bar{\psi}\chi\right)\right] \mathrm{d}x\mathrm{d}t\right\},$$

where $\delta[(4.10)]$, for example, is short hand notation for

$$\delta\left[(4.10)\right] = \delta\left[i\hbar\frac{\partial\psi}{\partial t} - \left(-\frac{\hbar^2}{2m}\nabla^2\psi + \left(g\left|\psi\right|^2 + V\right)\psi + \eta\right)\right].$$

Next we can rearrange the integrals which yields

$$K_{w}\left(\boldsymbol{\psi}_{b}, \boldsymbol{\bar{\psi}}_{b}, t_{b} | \boldsymbol{\psi}_{a}, \boldsymbol{\bar{\psi}}_{a}, t_{a}\right) = \iint \mathcal{D}\boldsymbol{\eta} \mathcal{D}\boldsymbol{\bar{\eta}} \iint_{\boldsymbol{\psi}(t_{a})=\boldsymbol{\psi}_{a}}^{\boldsymbol{\psi}(t_{b})=\boldsymbol{\psi}_{b}} \mathcal{D}\boldsymbol{\psi} \mathcal{D}\boldsymbol{\bar{\psi}} P\left[\boldsymbol{\eta}, \boldsymbol{\bar{\eta}}, \boldsymbol{\psi}, \boldsymbol{\bar{\psi}}\right] \delta\left[(4.10)\right] \delta\left[(4.11)\right]$$

where

$$P\left[\boldsymbol{\eta}, \bar{\boldsymbol{\eta}}, \boldsymbol{\psi}, \bar{\boldsymbol{\psi}}\right] = \iint \mathcal{D}\boldsymbol{\chi} \mathcal{D}\bar{\boldsymbol{\chi}} \exp\left\{-\frac{i}{\hbar} \iint \left(\left[\frac{g}{4}\left|\chi\right|^{2}\psi - \eta\right]\bar{\chi} + \left[\frac{g}{4}\left|\chi\right|^{2}\bar{\psi} - \bar{\eta}\right]\chi\right) \mathrm{d}x \mathrm{d}t\right\}.$$

The propagator can now be interpreted as an expectation value of a stochastic process generated by the additive noise field $\eta(x, t)$. The difficulty now resides in the expression for the noise probability P, which is still given by an unsolvable path integral. The fact that the noise probability explicitly depends on the field variables is also not very practical. A transformation of variables on χ and η , i.e.

$$\chi \to \left(\frac{4\hbar}{g |\psi|^4}\right)^{1/3} \psi \chi \text{ and } \eta \to \left(\frac{\hbar^2 g}{4 |\psi|^2}\right)^{1/3} \psi \eta,$$

however results in

$$K_{w}\left(\boldsymbol{\psi}_{b}, \boldsymbol{\bar{\psi}}_{b}, t_{b} | \boldsymbol{\psi}_{a}, \boldsymbol{\bar{\psi}}_{a}, t_{a}\right) = \iint \mathcal{D}\boldsymbol{\eta} \mathcal{D}\boldsymbol{\bar{\eta}} \iint_{\boldsymbol{\psi}(t_{a})=\boldsymbol{\psi}_{a}}^{\boldsymbol{\psi}(t_{b})=\boldsymbol{\psi}_{b}} \mathcal{D}\boldsymbol{\psi} \mathcal{D}\boldsymbol{\bar{\psi}} P\left[\boldsymbol{\eta}, \boldsymbol{\bar{\eta}}\right] \delta\left[(4.13)\right] \delta\left[(4.14)\right],$$

where

$$P[\boldsymbol{\eta}, \bar{\boldsymbol{\eta}}] = \iint \mathcal{D}\boldsymbol{\chi} \mathcal{D}\bar{\boldsymbol{\chi}} \exp\left\{-i \iint \left(\left[|\chi|^2 - \eta\right] \bar{\chi} + \left[|\chi|^2 - \bar{\eta}\right] \chi\right) \mathrm{d}x \mathrm{d}t\right\}$$
(4.12)

and the new Gross-Pitaevskii equation for ψ is

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + \left(g\left|\psi\right|^2 + V\right)\psi + \left(\frac{\hbar^2g}{4\left|\psi\right|^2}\right)^{1/3}\eta\psi, \qquad (4.13)$$

$$-i\hbar\frac{\partial\bar{\psi}}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\bar{\psi} + \left(g\left|\psi\right|^2 + V\right)\bar{\psi} + \left(\frac{\hbar^2g}{4\left|\psi\right|^2}\right)^{1/3}\bar{\eta}\bar{\psi}$$
(4.14)

Hence we can write the propagator as

$$K_{w}\left(\boldsymbol{\psi}_{b}, \bar{\boldsymbol{\psi}}_{b}, t_{b} | \boldsymbol{\psi}_{a}, \bar{\boldsymbol{\psi}}_{a}, t_{a}\right) = \iint \mathcal{D}\boldsymbol{\eta} \mathcal{D}\bar{\boldsymbol{\eta}} P\left[\boldsymbol{\eta}, \bar{\boldsymbol{\eta}}\right] \delta\left(\psi_{b} - \psi_{\eta}\left(t_{b} | \psi_{a}, t_{a}\right)\right) \delta\left(\bar{\psi}_{b} - \bar{\psi}_{\bar{\eta}}\left(t_{b} | \bar{\psi}_{a}, t_{a}\right)\right).$$
$$= \left\langle \delta\left(\psi_{b} - \psi_{\eta}\left(t_{b} | \psi_{a}, t_{a}\right)\right) \delta\left(\bar{\psi}_{b} - \bar{\psi}_{\bar{\eta}}\left(t_{b} | \bar{\psi}_{a}, t_{a}\right)\right) \right\rangle_{\eta}$$
(4.15)

where $\psi_{\eta}(t_b|\psi_a, \bar{\psi}_a, t_a)$ is the solution at time t_b of Eq.(4.13) with initial value ψ_a and $\bar{\psi}_{\bar{\eta}}$ is its conjugate field. This expression ought to be compared with expression (3.26) for the propagator of a system connected to a bath.

Now the remaining task is to calculate the noise probability function P. This can not be done exactly since the path integral is not Gaussian. If we neglect the third order terms in exactly the same way as in the truncated Wigner approximation we directly get that

$$P_{\text{TWA}}[\boldsymbol{\eta}, \bar{\boldsymbol{\eta}}] = \delta(\eta)\delta(\bar{\eta}),$$

which shows that up to this point we have just rewritten the propagator and we find back TWA under the same assumption. We can of course again expand around this result, which yields the complete perturbation series around the classical propagator

$$P\left[\boldsymbol{\eta}, \boldsymbol{\bar{\eta}}\right] \approx \delta(\eta)\delta(\bar{\eta}) + \iint \mathrm{d}x \mathrm{d}t \left[\partial_{\eta_{x,t}}^2 \delta(\eta)\partial_{\bar{\eta}_{x,t}} \delta(\bar{\eta}) + \partial_{\eta_{x,t}} \delta(\eta)\partial_{\bar{\eta}_{x,t}}^2 \delta(\bar{\eta})\right] + \dots \,.$$

Note that the noise probability itself is free of any physical parameters, it is simply a functional of η . The overall strength of the noise is thus contained in the prefactor $(\hbar^2 g/4n(x))^{1/3}$. It therefore becomes less and less important in the weak interaction and high density limit. Also note that path integral (4.12) does not contain differential operators any more. Consequently its effect is local in space-time and by considering the problem on a fixed rectangular space-time grid the path integral over the noise becomes a Riemann sum such that all the physics is governed by the ordinary integral

$$P\left[\eta_i, \bar{\eta}_i\right] = \iint \mathrm{d}\chi_i \mathrm{d}\bar{\chi}_i \exp\left(-i\epsilon\left(\left[|\chi_i|^2 - \eta_i\right]\bar{\chi}_i + \left[|\chi_i|^2 - \bar{\eta}_i\right]\chi_i\right)\right),\tag{4.16}$$

where $\epsilon = \Delta t \Delta^d x$ is the infinitesimal space-time volume and *i* denotes a lattice site in space time. Some analytical manipulations are necessary in order to convert this into a rapidly converging integral after which we can simply do this integral numerically. The result is depicted in Fig. (4.1). The noise amplitude again illustrates the exponential complexity of quantum mechanics. Although the noise amplitude decays rapidly outside the region arg $\eta'_i = \pm \pi/6$, it has more and more nodes with increasing $|\eta_i|$ inside the region $\phi \in (-\pi/6, \pi/6)$. This complements the discussion in chapter 2. The result also ought to be compared with the Markovian scattering rate of the weakly coupled polaron, depicted in Fig. (3.3). Figure (4.1) moreover illustrates that the effect of the noise on the classical propagator is never weak. The goodness of the classical propagator again depends on the initial state that is propagated.

4.2.2 Variational truncated Wigner approximation

Let us thus calculate the optimal effective classical Hamiltonian, associated with Hamiltonian (4.8), as presented in section 2.4.2. Since the previous result was formulated in terms of Poisson brackets it is invariant under a change of the underlying physical variables. We just have to replace our variables and the Hamiltonian for it, instead of $\{x, p\} = 1$ we have

$$\{\psi(x),\psi(x')\} = 0 = \{\bar{\psi}(x),\bar{\psi}(x')\} \text{ and } \{\psi(x),\bar{\psi}(x')\} = \delta(x-x').$$

Consequently the effective classical Hamiltonian satisfies

$$\{\{H_{\text{eff}}(\psi,\bar{\psi},t), f(\psi,\bar{\psi},t)\}, f(\psi,\bar{\psi},t)\} = \{\{H(\psi,\bar{\psi},t), f(\psi,\bar{\psi},t)\}_{M}, f(\psi,\bar{\psi},t)\}, \quad (4.17)$$

which is the field theory version of Eq. (2.50). Recall that, at present,

$$H = \int \left[\frac{\hbar^2}{2m} \nabla \bar{\psi}(x) \cdot \nabla \psi(x) + V(x) \left|\psi(x)\right|^2 + \frac{g}{2} \left|\psi^2(x)\right|^2\right] \mathrm{d}x.$$



Figure 4.1: Space-time sliced noise probability $P[\eta_i, \bar{\eta}_i]$. The dashed lines are guides for the eye, they represent Stokes lines in the saddle point approximation of $P[\eta_i, \bar{\eta}_i]$ at $\arg \eta'_i = \pm \pi/6$. Note that $\eta'_i = (4\epsilon^2/3)^{1/3} \eta_i$, where $\epsilon = \Delta t (\Delta x)^d$ is the infinitesimal space-time volume in d+1 dimensional space-time.

Consequently, since the Hamiltonian is at most quartic in the fields, the Moyal bracket truncates

$$\{H,f\}_M = \{H,f\} + \frac{g}{4} \int \mathrm{d}x \left(\psi(x) \frac{\delta^3 f(\psi,\bar{\psi})}{\delta\bar{\psi}\delta\psi^2} - \bar{\psi}(x) \frac{\delta^3 f(\psi,\bar{\psi})}{\delta\psi\delta\bar{\psi}^2}\right).$$

Since the Moyal bracket is expanded in the Poisson bracket plus a correction, it is natural to expand the trial Hamiltonian as

$$H_{\text{eff}} = H + H_c,$$

Again the equation (4.17) for H_c is rather hard to solve for a general distribution. Let us consider a coherent state $\hat{\rho} = |\psi_0(x)\rangle \langle \psi_0(x)|$ here. Then, similar to the discussion in section 2.4.2 the differential equation can be solved by Frobenius' method. There are many possible ways to rewrite the result, since the effective Hamiltonian is only determined up to a function which is in mutual involution with the Wigner distribution itself. A relatively simple way to write the result is the following:

$$H_{c} = \frac{g}{2} \int \left[\left(\psi \bar{\psi}_{0} \right)^{2} + \left(\bar{\psi} \psi_{0} \right)^{2} - |\psi|^{4} + 3 |\psi|^{2} + u \left(|\psi(x) - \psi_{0}(x)|^{2} \right) \right] \mathrm{d}x, \qquad (4.18)$$

where u(x) is a sufficiently differentiable function of x. Note that this has a peculiar effect on the effective classical Hamiltonian which now becomes

$$H_{\text{eff}} = \int \left[\frac{\hbar^2}{2m} \nabla \bar{\psi}(x) \cdot \nabla \psi(x) + \left(V(x) + \frac{3g}{2}\right) |\psi(x)|^2 + \frac{\bar{\Delta}(x)}{2} \psi^2(x) + \frac{\Delta(x)}{2} \bar{\psi}^2(x)\right] \mathrm{d}x.$$

where

$$\Delta(x) = g\psi_0^2(x). \tag{4.19}$$

The interaction term has completely been removed. Instead we find a quadratic Hamiltonian which has Bogoliubov pair terms. Similar to the quartic oscillator in section 2.4.2 one can check that the effective jump distribution around the effective Hamiltonian vanishes. Consequently the initial evolution of the classical trial state is identical to the true evolution. Moreover note that the characteristics satisfy

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + \left(V(x) + \frac{3g}{2}\right)\right]\psi(x) + \Delta(x)\bar{\psi}(x).$$

Consider the case where the field equals the expected field, i.e. $\psi = \psi_0$, which yields

$$i\hbar\frac{\partial}{\partial t}\psi_0(x,t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + \left(V(x) + \frac{3g}{2}\right)\right]\psi_0(x,t) + g\left|\psi_0\right|^2\psi_0(x,t).$$
(4.20)

Due to the definition (4.19) of Δ this is identical to the classical equation of motion up to a global phase factor. This phase factor is a consequence of Ehrenfest's theorem

$$i\hbar\frac{\partial}{\partial t}\left\langle\psi(x,t)\right\rangle = \left\langle\frac{\delta H(\psi,\bar{\psi})}{\delta\bar{\psi}(x)}\right\rangle$$

In agreement with the quartic oscillator, Ehrenfest's theorem is restored. Again, the theorem is restored in a curious way, by introducing terms in the effective Hamiltonian which at first sight have the wrong symmetry. In contrast to the quartic oscillator the effective classical Hamiltonian of a coherent state in the interacting bose gas is quadratic. This implies its equations of motion are still linear. For the quartic oscillator the trial evolution began to deviate from the real evolution because of the non-linearity of the classical equations of motion. The non-linearity would change the shape of the distribution, such that the asatz Gaussian trial state began to differ from the real evolved trial. In the present situation the linearity of the equations of motion will not distort the Gaussian state. As a consequence of the Bogoliubov pair terms the state however gets squeezed. The unsqueezed trial state is again different from the real squeezed state. The variational result is thus again correct up to second order.

Next I wish to note that in the present situation both the semiclassical and the variational truncated Wigner approximation give the same result in the thermodynamic limit, i.e. $N \to \infty$. The relative fluctuations in the density scale like $1/\sqrt{N}$, such that in the thermodynamic limit the Gaussian distribution function starts to look more and more like a point. In this limit only the description of the average density is relevant and one recovers the standard Gross-Pitaevskii equation for the order parameter $\psi_0(x,t)$. Recall that the true Gross-Pitaevskii equation and the effective Gross-Pitaevski equation (4.20) differ only by a global phase factor. This implies the two evolutions become equivalent as $N \to \infty$ since this phase can not be measured. However, the two approximations act completely different when a small incoherent part $g(\psi, \bar{\psi})$ is added to the coherent state distribution $f_0(\psi, \bar{\psi})$. Consider

$$f(\psi, \bar{\psi}) = (1 - \epsilon) f_0(\psi, \bar{\psi}) + \epsilon g(\psi, \bar{\psi}),$$

where ϵ is a small number. Within the semiclassical truncated Wigner approximation one would evolve the complete distribution $f(\psi, \bar{\psi})$ along the classical Gross-Pitaevskii trajectories. For the variational truncated Wigner approximation one needs to find the effective classical Hamiltonian associated with $f(\psi, \bar{\psi})$. In general we do not know this Hamiltonian because we do not know $g(\psi, \bar{\psi})$ but up to $O(\epsilon)$ we can approximate the effective Hamiltonian by the effective Hamiltonian of the coherent state f_0 . In the thermodynamic limit the evolution of the macroscopic coherent state f_0 would be equivalent in the semiclassical and the variational evolution but the evolution of the incoherent part $g(\psi, \bar{\psi})$ is completely different. Within the truncated Wigner approximation the latter is propagated along the Gross-Pitaevskii equation whereas the variational result recovers the standard Bogoliubov-de-Gennes result for fluctuations around a condensate.

The semiclassical truncated Wigner approximation should however recover the correct result in the classical, high temperature, limit. For the quartic oscillator the effective classical Hamiltonian and the real Hamiltonian become identical for $\sigma_p \to \infty$ and $\sigma_x \sigma_p \to \infty$, cf. Eq.(2.60). This implies the state must become highly mixed. In the present situation one can easily check by a simple substitution of variables in Eq. (4.18), that for the undisplaced but thermally populated vacuum the correction to the Hamiltonian becomes

$$H_{c} = -\frac{g}{2}\mu^{2} \int \left(|\psi|^{4} - 3|\psi|^{2} \right) \mathrm{d}x, \qquad (4.21)$$

where the purity $\mu \leq 1$. In the high temperature, $\mu \to 0$, limit the correction to the classical Hamiltonian vanishes and the variational result becomes equivalent to the truncated Wigner approximation.

The previous discussion clearly indicates the importance of the state itself in taking the classical limit. A fully coherent state has a non-interacting Hamiltonian with anomalous pair terms as classical limit whereas a fully thermal distribution has no pair terms but a renormalized interaction strength. Finding the effective Hamiltonian for an arbitrary state is an intractable problem, however the present effective Hamiltonian can be used as an ansatz effective Hamiltonian for the optimization of the classical evolution of states that are not Gaussian. Although one would like to parametrize the Hamiltonian with only a few parameters it ought to be clear that a good ansatz should at least include both of the previous results. I finally wish to note that the present discussion thereby supports Kleinert's critique [61] on the celebrated Hubbard-Stratanovich [57, 58] transformation. Not only do we provide a similar analysis, in the sense that we argue that the goodness of a specific expansion depends on the state of the system, we also provide a similar solution. Instead of introducing stochastic fields one should introduce an auxiliary classical Hamiltonian [18] for the system and link it to the state of the system.

Chapter 5

Concluding remarks and outlook

In this work we have studied Wigner's phase space formulation of quantum mechanics within Feynman's Lagrangian description of quantum mechanics. In principle most results can also be obtained in the Hamiltonian framework, using von Neumann's equation for the density matrix and solving the associated Wigner-Liouville equation by the method of characteristics. Although both methods are mathematically equivalent, the path integral approach offers a distinct advantage over the Hamiltonian approach for certain problems. It is also a more natural framework as it already avoids the use of operators from the start. Wigner's and Feynman's description of quantum mechanics moreover share their high affinity to classical mechanics. In the classical limit Wigner's description naturally results in a conservation of density on a Hamiltonian phase space flow. Feynman's description, on the other hand, constraints the solutions to the classical Euler-Lagrange equations of motion. In classical mechanics the Lagrangian and the Hamiltonian approach are linked trough the Legendre transformation. The Wigner-Weyl transformation plays a similar role in quantum mechanics. The quantum-classical correspondence is a recurring theme in this work. Several aspects of this correspondence are treated under different circumstances, in particular we discuss the classical limit in (i) single particle systems, (ii) systems connected to a bath and (iii) bosonic quantum field theories.

Chapter 2 introduces the Wigner function for a single particle system. An elementary introduction to Weyl ordering and Bopp operators is provided. Next, this section focuses on the propagation of an initial state in time. The propagator for the Wigner distribution is derived from Feynman's path integral and we explicitly show that the associated density matrix satisfies the Von Neumann equation for the density matrix. Chapter 2 furthermore contains an analytical treatment of the harmonic oscillator and double slit experiment. For the harmonic oscillator we recover the well known fact that classical and quantum dynamics are identical. I believe the combination of path integrals and Wigner's distribution provides a remarkably intuitive understanding of the double slit experiment. The analysis does not simply show that an interference pattern can be formed, it also includes the effect of diffraction. It moreover shows how the final interference pattern depends on the initial state, the shape of the slits and on the propagator in absence of geometrical constraints.

Considerable attention is finally devoted to the semiclassical truncated Wigner approximation. The full quantum dynamics is represented in terms of quantum jumps around the classical Hamiltonian phase space flow. Within the semiclassical truncated Wigner approximation one neglects the quantum jumps. Consequently the quantum dynamics is approximated by the classical evolution of the system. The justification for this expansion around the classical trajectory is based on the observation that every quantum jump carries an additional factor \hbar^2 . The overall goodness of the expansion is however unclear, since each successive term in the Moyal expansion contains higher derivatives of both the distribution and the Hamiltonian. In that respect it is important to note that the Euler-Lagrange equations for the saddle-point expansion of the Wigner distribution propagator differ from the classical equations of motion, unless the problem is harmonic. Although the classical equation of motion does lie on a saddlepoint, there are infinitely many others such that it has zero measure in the semiclassical path integral. The final part of chapter 2 shows that a modified classical phase space evolution exists around which the overall quantum fluctuations are smaller. A method to extract the Hamiltonian that generates this motion is presented.

In chapter 3 the obtained result is extended by computing the path integral for the propagator of the reduced Wigner function of a system coupled to an external quantum system. The focus is again on a single particle system but this time connected to a set of harmonic oscillator such that the dynamics of the bath is analytically tractable. As long as the coupling is bilinear the dynamics of the reduced distribution is still analytically tractable. In the remaining part of chapter 3 the discussion is devoted to the polaron problem. Due to the non-linearity of the coupling between the system and the bosonic bath, the reduced system dynamics can not be solved analytically. A perturbation theory for the propagator is developed. Considerable attention is again devoted to the classical limit. It is shown under which approximations the resulting equation of motion reduces to the linear Wigner-Boltzmann equation where the collision integral is given by Fermi's golden rule. The section finally contains an alternative method to calculate the linear response coefficient of the coupled system. The method is based on a systematic truncation of the Liouville equation for the reduced distribution function. Explicit expressions for the conductivity of the Fröhlich polaron are presented. At present the method can only be justified in the weak-coupling, low-temperature regime. Further research ought to be concerned with an extension to the strong-coupling and/or high-temperature regime. The possibility of solving the reduced Wigner Liouville equation numerically should moreover be explored. If successful it might rival diagrammatic Monte Carlo calculations of the linear response coefficients.

Chapter 4 finally focusses on coherent state Wigner distributions of bosonic quantum fields. In complete agreement with the result in first quantization, we find that for all harmonic problems, only the classical trajectory contributes to the path integral. Except in this case the classical limit yields the Schrödinger equation for the fields rather than Newtonian equations of motion for the point particle. For non-harmonic, interacting, problems the problem is in general not analytically solvable. We again present a perturbation theory around the classical trajectory. This time, we however adopt a stochastic differential equation approach. It again shows that the goodness of the expansion around the classical trajectory depends strongly on the initial state of the system. The analysis moreover shows that the quantum noise can neither be considered additive nor multiplicative. The final part of the section is concerned with the optimal effective classical Hamiltonian of a bosonic gas where the particles interact trough contact interaction. The effective Hamiltonian is presented both for a fully coherent state and a state with non-minimal uncertainty. In contrast to the truncated Wigner approximation the present method recovers the standard Bogoliubov-de-Gennes result for fluctuations around a condensate. Further research in this area focusses on an extension to fermionic fields and a more profound understanding of the relation between the present method and Kleinert's variational perturbation theory [18, 62].
Scientific contributions

Refereed journal publications

- D. Sels, F. Brosens, Self-energy correction to dynamic polaron response, Phys. Rev. E 89, 042110 (2014), doi:10.1103/PhysRevE.89.042110
- D. Sels, F. Brosens, Variational Truncated Wigner Approximation, Phys. Rev. E 89, 042107 (2014), doi:10.1103/PhysRevE.89.042107
- D. Sels, F. Brosens, Truncated phase-space approach to polaron response, Phys. Rev. E 89, 012124 (2014), doi: 10.1103/PhysRevE.89.012124
- 4. D. Sels, F. Brosens, Wigner distribution functions for complex dynamical systems : the emergence of the Wigner-Boltzmann equation, Phys. Rev. E 88:4 042101, (2013), doi: 10.1103/PhysRevE.88.042101
- D. Sels, F. Brosens, W. Magnus, Wigner distribution functions for complex dynamical systems : a path integral approach, Physica: A. 392:2, p. 326-335, (2013), doi: 10.1016/:j.physa.2012.09.007
- D. Sels, F. Brosens, W. Magnus, On the path integral representation of the Wigner function and the Barker-Murray ansatz, Physics letters: A 376:6/7, p. 809-812, (2012), doi: 10.1016/j.physleta.2012.01.020
- D. Sels, F. Brosens, W. Magnus, Classical trajectories: A powerful tool for solving tunneling problems, Physica: A: 391:1/2, p. 78-81, (2012), doi: 10.1016/j.physa.2011.08.030
- D. Sels, B. Sorée, G. Groeseneken, Quantum ballistic transport in the junctionless nanowire pinch-off field effect transistor, Journal of computational electronics 10:1, p. 216-22, (2011), doi: 10.1007/s10825-011-0350-2

Chapters in Books

B. Sorée, A.-T. Pham, D. Sels, W. Magnus, *The junctionless nanowire transistor*, CMOS nanoelectronics : innovative devices, architectures, and applications, - ISBN 9789814364027
 - S.I., Pan Stanford, (2012)

Invited lectures

- 1. Path integrals in phase space, Theory at sea 2014, Oostende, 14-15 April 2014
- 2. Wigner distribution functions for complex dynamical systems, Condensed matter theory seminar series, Boston University, Boston, Oct. 16 2013
- 3. Quantum transport and classical trajectories, MSP meeting, imec, Leuven, Feb. 03 2011
- 4. Dynamics of 2D topological insulators: quantum (spin) Hall effect, MSP meeting, imec, Leuven, Mar. 08 2011

Conference contributions

- 1. D. Sels, A phase-space approach to thermalization, Stellenbosch Workshop on Equilibration and thermalization in quantum system, Stellenbosch, April, 2013. Oral contribution
- D. Sels, F. Brosens, W. Magnus, Wigner distribution functions for complex dynamical systems: a path integral approach, MAR13 Meeting of The American Physical Society, Baltimore, March, 2013. Oral contribution
- 3. D. Sels, F. Brosens, W. Magnus, *Phase-space dynamics of the quantum Hall state*, Belgian Physical Society General scientific meeting, Brussel, 30 May, 2012. *Oral contribution*
- D. Sels, F. Brosens, W. Magnus, B. Sorée, *Phase-space dynamics of 2D topological insula*tors, Belgian Physical Society General scientific meeting, Brussels, 30 May, 2012. *Poster,* Third price at 'European Physics Journal best poster award'.
- 5. W. Magnus, F. Brosens, D. Sels, *Classical phase space trajectories: powerful allies for studying Wigner function based quantum transport*, 37th Conference of the Middle European Cooperation in Statistical Physics, March 18-22, 2012. *Oral contribution*
- D. Sels, F. Brosens, W. Magnus, B. Sorée, Wigner path integral solution for the integer quantum Hall effect, MAR12 Meeting of The American Physical Society, Boston, March, 2012. Oral contribution
- B. Sorée, A.-T. Pham, D. Sels, W. Magnus, *The junctionless nanowire transistor: trans*port properties, Belgian Physical Society General scientific meeting, Namur, 25 May, 2011. *Poster*
- 8. B. Sorée, A.-T. Pham, D. Sels, A. De Keersgieter, W. Magnus, *Junctionless nanowire field-effect transistor versus inversion mode devices*, MAR11 Meeting of The American Physical Society, Dallas, March, 2011. *Oral contribution*
- D. Sels, B. Sorée, G. Groeseneken, Single dopant effects in ballistic nanowire transistors, Nanoelectronics days 2010, Aachen, October 04-07, 2010. Poster
- B. Sorée, D. Sels, A. De Keersgieter, W. Magnus, Junctionless nanowire field-effect transistor versus inversion mode devices, Nanoelectronics days 2010, Aachen, October 04-07, 2010. Oral contribution
- 11. D. Sels, B. Sorée, G. Groeseneken, 2-D rotational invariant multi sub band Schrödinger-Poisson solver to model nanowire transistors, 14th International Workshop on Computational Electronics, Pisa, 2010. Poster

Appendix A

Wigner propagator for quadratic potentials

In this appendix the propagator (2.34) of the Wigner function for quadratic potentials of the form

$$V_{\text{quad}}(x,t) = a(t) + b(t)x + c(t)x^2$$
 (A.1)

is derived from the well known [23] Feynman propagator $K_{\text{quad}}(x_b, t_b | x_a, t_a)$ for this type of potentials:

$$K_{\text{quad}}\left(x_{b}, t_{b} | x_{a}, t_{a}\right) = \sqrt{\frac{m}{2\pi i \hbar g\left(t_{b}, t_{a}\right)}} \exp\left(\frac{i}{\hbar} S_{\text{quad}}\left(x_{b}, t_{b} | x_{a}, t_{a}\right)\right),\tag{A.2}$$

$$S_{\text{quad}}(x_b, t_b | x_a, t_a) = \int_{t_a}^{t_b} \left(\frac{m}{2} \dot{x}^2 - a(t) - b(t) x - c(t) x^2\right) \mathrm{d}t, \tag{A.3}$$

where $S_{\text{quad}}(x_b, t_b | x_a, t_a)$ is the action of the system along a classical trajectory from (x_a, t_a) to (x_b, t_b) , to be determined from the classical equation of motion

$$m\ddot{x} + 2c(t)x = -b(t) \text{ with } \begin{array}{l} x(t_a) = x_a, \\ x(t_b) = x_b. \end{array}$$
(A.4)

The function $g(t_b, t_a)$ only depends on the initial and final time, and is independent of the positions and momenta. It is the solution of the differential equation

$$\left(m\frac{d^2}{dt^2} + 2c\left(t\right)\right)g\left(t, t_a\right) = 0 \text{ with } \frac{g\left(t_a, t_a\right) = 0,}{\frac{d}{dt}g\left(t, t_a\right)\Big|_{t=t_a}} = 1.$$
(A.5)

For general time dependence of c(t), these differential equations rarely have a solution in closed form, but it is sure that two linearly independent solutions, say $x_1(t)$ and $x_2(t)$, of the homogeneous equations exist:

$$m\ddot{x}_{1,2} + 2c(t) x_{1,2} = 0.$$
(A.6)

Their Wronskiaan $\frac{dx_1(t)}{dt}x_2(t) - \frac{dx_2(t)}{dt}x_1(t)$ is independent of t, because (A.6) reveals that its time derivative is zero

$$\frac{dx_1(t)}{dt}x_2(t) - \frac{dx_2(t)}{dt}x_1(t) = W \text{ independent of } t.$$
(A.7)

Since $g(t, t_a)$ is also a solution of the *homogeneous* differential equation (A.6), it is a linear combination of $x_1(t)$ and $x_2(t)$. Taking the boundary conditions into account it becomes

$$g(t, t_a) = \frac{h(t, t_a)}{W} \text{ with } h(s, t) = x_1(s) x_2(t) - x_2(s) x_1(t).$$
 (A.8)

If one imposes that the solution of the homogeneous differential equation (A.6) exhausts the boundary conditions at t_a and t_b , the trajectory x(t) is of the form

$$x(t) = \frac{h(t, t_b)}{h(t_a, t_b)} x_a + \frac{h(t_a, t)}{h(t_a, t_b)} x_b + x_p(t),$$
(A.9)

where the particular solution $x_p(t)$ has to satisfy the boundary conditions $x_p(t_a) = 0 = x_p(t_b)$. It is easily found by the variation of parameters method, with the result:

$$x_{p}(t) = -\frac{h(t,t_{b})}{h(t_{a},t_{b})} \int_{t_{a}}^{t} \frac{b(s)}{m} \frac{h(t_{a},s)}{W} \,\mathrm{d}s - \frac{h(t_{a},t)}{h(t_{a},t_{b})} \int_{t}^{t_{b}} \frac{b(s)}{m} \frac{h(s,t_{b})}{W} \,\mathrm{d}s.$$
(A.10)

It is fairly easy to calculate the initial and final velocities $\dot{x}_{a,b}$, which are of particular relevance below:

$$\dot{x}_{a} = \frac{1}{h\left(t_{a}, t_{b}\right)} \left(x_{a} \frac{\partial h\left(t_{a}, t_{b}\right)}{\partial t_{a}} - x_{b}W + \int_{t_{a}}^{t_{b}} \frac{b\left(s\right)}{m} h\left(s, t_{b}\right) \mathrm{d}s \right),$$
(A.11)

$$\dot{x}_{b} = \frac{1}{h\left(t_{a}, t_{b}\right)} \left(x_{a}W + x_{b} \frac{\partial h\left(t_{a}, t_{b}\right)}{\partial t_{b}} - \int_{t_{a}}^{t_{b}} \frac{b\left(s\right)}{m} h\left(t_{a}, s\right) \,\mathrm{d}s \right).$$
(A.12)

Applying an integration by parts $\int \dot{x}^2 dt = x\dot{x} - \int x\ddot{x}dt$ in the kinetic contribution to the classical action, it can be rewritten as

$$S_{\text{quad}}(x_b, t_b | x_a, t_a) = \frac{m}{2} \left([x \dot{x}]_{t=t_a}^{t=t_b} - \int_{t_a}^{t_b} \frac{b(t)}{m} x(t) \, \mathrm{d}t \right)$$

$$= \frac{m}{h(t_a, t_b)} \left(\frac{x_b^2 \frac{dh(t_a, t_b)}{dt_b} - x_a^2 \frac{dh(t_a, t_b)}{dt_a}}{2} + W x_a x_b - x_b \int_{t_a}^{t_b} \frac{b(s)}{m} h(t_a, s) \, \mathrm{d}s - x_a \int_{t_a}^{t_b} \frac{b(s)}{m} h(s, t_b) \, \mathrm{d}s \right) - \frac{1}{2} \int_{t_a}^{t_b} b(s) x_p(s) \, \mathrm{d}s, \quad (A.13)$$

where the boundary velocities and the homogenous contribution x(t) have been filled out.

In the propagator for harmonic interactions of the form (A.1), only terms linear in $\xi_{a,b}$ survive in the exponent, and one is left with

$$\begin{aligned}
K_w \left(x_b, p_b, t_b | x_a, p_a, t_a\right) &= \frac{mW}{\left(2\pi\hbar\right)^2 h\left(t_b, t_a\right)} \times \\
&\times \int \exp\left(\frac{i}{\hbar}\xi_b \left(-p_b + \frac{m}{h\left(t_a, t_b\right)} \left(x_a W + x_b \frac{dh\left(t_a, t_b\right)}{dt_b} - \int_{t_a}^{t_b} \frac{b\left(s\right)}{m} h\left(t_a, s\right) \, \mathrm{d}s\right)\right)\right) \, \mathrm{d}\xi_b \\
&\times \int \exp\left(\frac{i}{\hbar}\xi_a \left(p_a - \frac{m}{h\left(t_a, t_b\right)} \left(x_a \frac{dh\left(t_a, t_b\right)}{dt_a} - x_b W + \int_{t_a}^{t_b} \frac{b\left(s\right)}{m} h\left(s, t_b\right) \, \mathrm{d}s\right)\right)\right) \, \mathrm{d}\xi_a, \quad (A.14)
\end{aligned}$$

where the remaining integrals are δ -functions. Taking the results for the boundary velocities into account, one thus readily finds

$$\begin{array}{lll}
K_{w}\left(x_{b}, p_{b}, t_{b} | x_{a}, p_{a}, t_{a}\right) &= & \delta\left(x_{b} - x_{cl}\left(t_{b} | x_{a}, p_{a}, t_{a}\right)\right) \delta\left(p_{b} - p_{cl}\left(t_{b} | x_{a}, p_{a}, t_{a}\right)\right) \\
&= & \delta\left(x_{a} - x_{cl}\left(t_{a} | x_{b}, p_{b}, t_{b}\right)\right) \delta\left(p_{a} - p_{cl}\left(t_{a} | x_{b}, p_{b}, t_{b}\right)\right)
\end{array}$$

which is the desired result (2.34, 2.35).

Appendix B

Green's function of the effective Hamiltonian

In this appendix we present a scheme to find the effective classical Hamiltonian of a general Gaussian Wigner distribution.

$$f(x,p) = \frac{1}{2\pi\sqrt{\det \boldsymbol{\sigma}}} \exp\left(-\left(\mathbf{r} - \mathbf{r}_0\right)^T \boldsymbol{\sigma}^{-1} \left(\mathbf{r} - \mathbf{r}_0\right)\right),$$

where $\mathbf{r}^T = (x, p)$, \mathbf{r}_0 denotes the average phase space point $\mathbf{r}_0^T = (x_0, p_0)$ and $\boldsymbol{\sigma}$ is the covariance matrix. Note that $\sqrt{\det \boldsymbol{\sigma}} \geq \hbar/2$ in order to be in agreement with Heisenbergs uncertainty principle. Recall the effective Hamiltonian satisfies

$$\{\{H_{\text{eff}}(x,p), f(x,p)\}, f(x,p)\} = \{\{H(x,p), f(x,p)\}_M, f(x,p)\}.$$
(B.1)

with H(x, p) the real Hamiltonian. In order to simplify the derivation, let us first do a canonical transformation to center the Gaussian state around the origin. Such a transformation leaves both the Poisson and the Moyal bracket invariant since it is composed of two unitary transformations, i.e. a shift operation

followed by a rotation

$$\mathbf{U}^T \mathbf{r} \rightarrow \mathbf{r}$$

 $\mathbf{r} - \mathbf{r}_0 \rightarrow \mathbf{r},$

where

$$\boldsymbol{\sigma} = \mathbf{U} \begin{pmatrix} \sigma_x^2 & 0\\ 0 & \sigma_p^2 \end{pmatrix} \mathbf{U}^T.$$

The remaining Gaussian state is now centered around the origin, consequently we find

$$\{f, \{H_{\text{eff}}, f\}\} = f^2 \left(-\frac{x^2}{\sigma_x^4} \frac{\partial}{\partial p^2} - \frac{p^2}{\sigma_p^4} \frac{\partial^2}{\partial x^2} + \frac{2xp}{\sigma_x^2 \sigma_p^2} \frac{\partial^2}{\partial x \partial p} + \frac{1}{\sigma_p^2 \sigma_x^2} \left(x \frac{\partial}{\partial x} + p \frac{\partial}{\partial p} \right) \right) H_{\text{eff}}(x, p).$$

Consequently Eq.(B.1) can be written as

$$\left(-\frac{x^2}{\sigma_x^4}\frac{\partial}{\partial p^2} - \frac{p^2}{\sigma_p^4}\frac{\partial^2}{\partial x^2} + \frac{2xp}{\sigma_x^2\sigma_p^2}\frac{\partial^2}{\partial x\partial p} + \frac{1}{\sigma_p^2\sigma_x^2}\left(x\frac{\partial}{\partial x} + p\frac{\partial}{\partial p}\right)\right)H_{\text{eff}}(x,p) = Q(x,p),$$

where $Q = f^{-2} \{ \{H, f\}_M, f \}$. Let us finally put everything in dimensionless variables

$$\frac{x}{\sigma_x} \to x, \quad \frac{p}{\sigma_p} \to p.$$

Then we arrive at

$$\left(-x^2\frac{\partial^2}{\partial p^2} - p^2\frac{\partial^2}{\partial x^2} + 2xp\frac{\partial^2}{\partial x\partial p} + \left(x\frac{\partial}{\partial x} + p\frac{\partial}{\partial p}\right)\right)H_{\text{eff}}(x,p) = Q'(x,p),$$

where $Q'(x,p) = \sigma_p^2 \sigma_x^2 Q(x,p)$. Consequently we can find the solution for arbitrary Hamiltonian if we have the Green function

$$\left(-x^2\frac{\partial^2}{\partial p^2} - p^2\frac{\partial^2}{\partial x^2} + 2xp\frac{\partial^2}{\partial x\partial p} + \left(x\frac{\partial}{\partial x} + p\frac{\partial}{\partial p}\right)\right)G(x, p|x', p') = \delta(x - x')\delta(p - p').$$

Although none of the above transformations is strictly necessary they significantly simplify the remaining calculation. The homogeneous equation has now become invariant under exchange of x and p, such that it is instructive to go to polar coordinates

$$\begin{array}{rcl} x &=& r\cos\phi, \\ p &=& r\sin\phi. \end{array}$$

After some algebra we find the following equation for Green's function

$$-\frac{\partial^2}{\partial \phi^2} G(r,\phi|r',\phi') = \frac{1}{r} \delta(r-r') \delta(\phi-\phi').$$

The remaining problem is separable and does not contain any radial differential operators any more such that we immediately find

$$G(r,\phi|r',\phi') = \frac{1}{r}\delta(r-r')\Phi(\phi-\phi'),$$

where

$$-\frac{\partial^2}{\partial \phi^2} \Phi(\phi) = \delta(\phi).$$

This equation can now be solved under the condition that Φ is a 2π periodic function. This condition can easily be implemented by expanding the function in a complete set of 'angular momentum' states. The sum can afterwords be done and it yields a dilogarithmic function. The arguments are complex exponentials such that the result can be written in terms of Bernoulli polynomials of order 2. Any constant can be added to the result such that we eventually find

$$\Phi(\phi) = \pi \left[\left(\frac{\phi}{2\pi} \right) - \left(\frac{\phi}{2\pi} \right)^2
ight].$$

In order to find the effective Hamiltonian we should convolve this Greens function with Q'(x, p). This gives us the effective Hamiltonian in the new scaled, rotated and shifted reference frame. As a final step we should undo all these transformations to obtain the effective classical Hamiltonian in the original frame.

Appendix C

Polaron Mobility

In this appendix we re-examine the relaxation time approximation and the FHIP approximation in the language of Wigner distributions.

C.1 Relaxation time approximation

The purpose of this Appendix is to explain the discrepancy in (3.54) by a factor of 3 between the dc conductivity of the Fröhlich polaron which we derived in (3.53), as compared to the Kadanoff result [41]. Since we are only concerned with stationary values we consider the linearized Liouville equation for the reduced Wigner function, i.e. the true self energy is approximated by the free particle self energy. Using $\int_{-\infty}^{t} \cos((t-s)a) ds = \pi \delta(a)$ one easily derives that its stationary version is a Boltzmann equation

$$e\mathbf{E} \cdot \frac{df(\mathbf{p})}{d\mathbf{p}} = -\Pi(\mathbf{p}) f(\mathbf{p}) + \int \Pi(\mathbf{p} + \hbar \mathbf{k} \to \mathbf{p}) f(\mathbf{p} + \hbar \mathbf{k}) d\mathbf{k}, \qquad (C.1)$$

where we adopt an analogous notation as by Devreese and Evrard in [56], and define

$$\Pi\left(\mathbf{p}+\hbar\mathbf{k}\to\mathbf{p}\right) = \frac{V\left|\gamma\left(k\right)\right|^{2}}{\left(2\pi\right)^{2}\hbar} \left(\begin{array}{c} \left(n_{B}\left(\omega_{k}\right)+1\right)\delta\left(\frac{\left(\mathbf{p}+\hbar\mathbf{k}\right)^{2}-\mathbf{p}^{2}}{2m}-\hbar\omega_{k}\right)\right)\\ +n_{B}\left(\omega_{k}\right)\delta\left(\frac{\left(\mathbf{p}+\hbar\mathbf{k}\right)^{2}-\mathbf{p}^{2}}{2m}+\hbar\omega_{k}\right)\end{array}\right), \quad (C.2)$$

$$\Pi(\mathbf{p}) = \int \Pi(\mathbf{p} \to \mathbf{p} + \hbar \mathbf{k}) \, d\mathbf{k}. \tag{C.3}$$

Because the unperturbed reduced Wigner distribution function at sufficiently low temperature peaks around $\mathbf{p} = 0$, one might argue that the dominant term in the right hand side is given by $-f(\mathbf{p}) \lim_{\mathbf{p} \to \mathbf{0}} \Pi(\mathbf{p})$, which gives rise to a relaxation time approximation (RTA):

$$e\mathbf{E} \cdot \frac{df(\mathbf{p})}{d\mathbf{p}} \approx -\frac{f(\mathbf{p})}{\tau} \text{ with } \tau = \frac{1}{\lim_{\mathbf{p} \to \mathbf{0}} \Pi(\mathbf{p})}.$$

The first moment of this equation with respect to \mathbf{p} , taking (3.44) into account, then immediately leads to

$$\mathbf{J} = \lim_{\mathbf{p} \to 0} \frac{e^2/m}{\Pi(\mathbf{p})} \mathbf{E} \text{ hence } \sigma_{DC} = \lim_{\mathbf{p} \to 0} \frac{e^2/m}{\Pi(\mathbf{p})}$$

For the Fröhlich polaron, with the constant frequency $\omega_k = \omega_{LO}$ and the electron-phonon coupling (3.51), the corresponding function $\Pi_{\text{Fröhlich}}(\mathbf{p})$ can easily be calculated in closed form:

$$\Pi_{\text{Fröhlich}}\left(\mathbf{p}\right) = 2\alpha\omega_{LO}\frac{\sqrt{2m\hbar\omega_{LO}}}{p} \left(\begin{array}{c} \left(n_B(\omega_{LO})+1\right)\Theta\left(\hbar\omega_{LO}<\frac{p^2}{2m}\right)\operatorname{arccosh}\frac{p}{\sqrt{2m\hbar\omega_{LO}}}\\ +n_B(\omega_{LO})\operatorname{arcsinh}\frac{p}{\sqrt{2m\hbar\omega_{LO}}}\end{array}\right),$$

This simple relaxation time approximation thus immediately gives the Kadanoff conductivity for the Fröhlich polaron:

$$\sigma_{DC}_{\text{Kadanoff}} = \lim_{\mathbf{p} \to 0} \frac{e^2/m}{\prod_{\text{Fröhlich}} (\mathbf{p})} \approx \frac{1}{2} \frac{e^2}{m \alpha \omega_{LO}} e^{\beta \hbar \omega_{LO}}.$$

However, the neglect of the integral term in (C.1) is an unwarranted approximation, essentially because it violates the particle number conservation. Indeed, consider the first moment of (C.1) with respect to \mathbf{p} :

$$e\mathbf{E} = \int \mathbf{p}\Pi(\mathbf{p}) f(\mathbf{p}) d\mathbf{p} - \int \int \mathbf{p}\Pi(\mathbf{p} + \hbar \mathbf{k} \to \mathbf{p}) f(\mathbf{p} + \hbar \mathbf{k}) d\mathbf{k} d\mathbf{p}.$$

By the substitution $\mathbf{p} + \hbar \mathbf{k} \to \mathbf{p}$ in the last term, interchanging $\mathbf{k} \leftrightarrow -\mathbf{k}$ and using the definition (3.48), the terms in $\Pi(\mathbf{p})$ cancel against each other, and one is left with

$$eE = -\mathbf{1}_{E} \cdot \int \int \hbar \mathbf{k} \Pi \left(\mathbf{p} \to \mathbf{p} + \hbar \mathbf{k} \right) f \left(\mathbf{p} \right) d\mathbf{k} d\mathbf{p},$$

which shows that the in-scattering rate can not be neglected.

At sufficiently low temperature, the distribution function peaks at $\mathbf{\bar{p}} = m\mathbf{J}/e$ which is indeed near $\mathbf{p} = \mathbf{0}$ since $\mathbf{\bar{p}} \propto \mathbf{E} \rightarrow \mathbf{0}$. Replacing $f(\mathbf{p})$ by $\delta(\mathbf{p}-m\mathbf{J}/e)$ then gives

$$eE = -\mathbf{1}_E \cdot \int \hbar \mathbf{k} \Pi \left(\frac{m\mathbf{J}}{e} \to \frac{m\mathbf{J}}{e} + \hbar \mathbf{k} \right) d\mathbf{k}.$$
(C.4)

For the Fröhlich polaron (3.51), the evaluation of this integral is elementary and results in:

$$eE = m\omega_{LO}\alpha\sqrt{2}\sqrt{\frac{\hbar\omega_{LO}}{m}}\frac{2e^2}{mJ^2} \times \left(\begin{array}{c} \left(n_B\left(\omega_{LO}\right) + 1\right)\Theta\left(\hbar\omega_{LO} < \frac{mJ^2}{2e^2}\right)\left(\frac{\sqrt{mJ}}{\sqrt{2e}}\sqrt{\frac{mJ^2}{2e^2}} - \hbar\omega_{LO} + \hbar\omega_{LO}\operatorname{arccosh}\left(\frac{J}{e}\frac{\sqrt{m}}{\sqrt{2\hbar\omega_{LO}}}\right)\right) \\ + n_B\left(\omega_{LO}\right)\left(\frac{\sqrt{mJ}}{\sqrt{2e}}\sqrt{\frac{mJ^2}{2e^2}} + \hbar\omega_{LO} - \hbar\omega_{LO}\operatorname{arcsinh}\left(\frac{J}{e}\frac{\sqrt{m}}{\sqrt{2\hbar\omega_{LO}}}\right)\right) \\ \end{array} \right).$$
(C.5)

Keeping linear response in mind, it is obvious that this expression is only needed tot first order in J = O(E), such that the emission term does not contribute at sufficiently low temperature. The result is

$$eE = \frac{2}{3}m\omega_{LO}\alpha n_B\left(\omega_{LO}\right)\frac{J}{e} + O\left(J^3\right),\tag{C.6}$$

which is fully consistent with the conductivity (3.53) derived in section (3.4).

C.2 FHIP with Wigner distributions

In this section we present a calculation in the spirit of the FHIP approximation but using our phase space approach. It was shown in section 3.3 how the path integral for the reduced Wigner function leads to the Liouville equation (3.34). The path integral for the reduced Wigner function is just the Weyl transform of the path integral for the density matrix used by FHIP. The basic approach in FHIP is to expand the action around Feynman's linear polaron model, rather than around the free particle. In terms of the distribution function this means that

$$f(\mathbf{p},t) = f_0(\mathbf{p},t) + f_1(\mathbf{p},t),$$
 (C.7)

where f_0 is a variational time dependent Wigner function which can be found by propagating the initial distribution along a certain, so far free to choose, linear model. Similar as for the linear response at weak coupling (i.e., to first order in the deviation from the free particle), we now consider linear response to first order in the deviation from the Feynman polaron model, which means that

$$\left(\frac{\partial}{\partial t} + e\mathbf{E}\cdot\nabla_p\right)f_1(\mathbf{p},t) = g_0(\mathbf{p},t),\tag{C.8}$$

where $g_0(\mathbf{p}, t)$:

$$g_{0}(\mathbf{p},t) = -\left(\frac{\partial}{\partial t} + e\mathbf{E}(t)\cdot\nabla\right)f_{0}(\mathbf{p},t)$$

$$+\sum_{\mathbf{k}}\frac{2\left|\gamma\left(k\right)\right|^{2}}{\hbar^{2}}\int_{-\infty}^{t}\left(\begin{array}{c}f_{0}\left(\mathbf{p}+\hbar\mathbf{k},s\right)\left(\begin{array}{c}\left(n_{B}\left(\omega_{k}\right)+1\right)\cos\left(\left(t-s\right)\left(\mathbf{k}\cdot\frac{\mathbf{p}+\frac{\hbar\mathbf{k}}{2}}{m}-\omega_{k}\right)\right)\right)\\+n_{B}\left(\omega_{k}\right)\cos\left(\left(t-s\right)\left(\mathbf{k}\cdot\frac{\mathbf{p}+\frac{\hbar\mathbf{k}}{2}}{m}+\omega_{k}\right)\right)\\-f_{0}\left(\mathbf{p},s\right)\left(\begin{array}{c}\left(n_{B}\left(\omega_{k}\right)+1\right)\cos\left(\left(t-s\right)\left(\mathbf{k}\cdot\frac{\mathbf{p}+\frac{\hbar\mathbf{k}}{2}}{m}-\omega_{k}\right)\right)\\+n_{B}\left(\omega_{k}\right)\cos\left(\left(t-s\right)\left(\mathbf{k}\cdot\frac{\mathbf{p}+\frac{\hbar\mathbf{k}}{2}}{m}-\omega_{k}\right)\right)\end{array}\right)\right)\right)ds.$$
(C.9)

The time dependence of the distribution function f_1 follows the classical equation of motion, and consequently

$$f_1(\mathbf{p},t) = \int_{-\infty}^t g_0\left(\mathbf{p} - \int_{t'}^t e\mathbf{E}(s)\mathrm{d}s, t'\right)\mathrm{d}t'.$$

Because of the particle number conservation of the trial distribution, and due to the linearity of the classical equation of motion, the expected current density of the perturbation around the model becomes

$$\mathbf{J}_1(t) = \frac{e}{m} \int \mathbf{p} f_1(\mathbf{p}, t) \mathrm{d}\mathbf{p} = \frac{e}{m} \int_{-\infty}^t \int \mathbf{p} g_0(\mathbf{p}, t') \mathrm{d}\mathbf{p} \mathrm{d}t'.$$
 (C.10)

The total current density is consequently given by

$$\mathbf{J}(t) = \mathbf{J}_0(t) + \mathbf{J}_1(t),$$

where $\mathbf{J}_0(t)$ is the current density of the model distribution function. In terms of Feynman's variational parameters w and v, Feynman's model distribution function reads

$$f_0(\mathbf{p},t) = \left(\frac{\beta}{2m\pi}\right)^{3/2} \exp\left(-\frac{\beta}{2m}\left(\mathbf{p} - \frac{w^2}{v^2}\int_{-\infty}^t e\mathbf{E}(s)\mathrm{d}s - \frac{v^2 - w^2}{v^2}\int_{-\infty}^t e\mathbf{E}(s)\cos v(t-s)\mathrm{d}s\right)^2\right)$$

provided we assume the model to be initially in canonical equilibrium at an effective temperature equal to the real inverse temperature β . At this point the present discussion differs from that of FHIP, where the initial state of the model is assumed to be a product state of the oscillators and the particle. It is argued by FHIP that the product state ansatz is admissible because "... In the past only the oscillators were in thermal equilibrium at β^{-1} . As a result of the coupling the system will come very quickly to thermal equilibrium at the same temperature. [42]" Although this might be true for the real system, it does not apply to the model. Because of the linearity of the model it will never thermalize. Consequently, the reduced model distribution function will endlessly oscillate even in the absence of an electric field. In contrast, the present model distribution is the exact stationary distribution of the reduced Liouville equation in the absence of an electric field, as discussed in section 3.4. It should however also be noted that, as a consequence of the same linearity, the expected model current density

$$\mathbf{J}_{0}(t) = \frac{w^{2}}{v^{2}} \int_{-\infty}^{t} \frac{e^{2}\mathbf{E}(s)}{m} ds + \frac{v^{2} - w^{2}}{v^{2}} \int_{-\infty}^{t} \frac{e^{2}\mathbf{E}(s)}{m} \cos v(t - s) ds,$$

is not affected by the change in initial state, in contrast to the correction $\mathbf{J}_1(t)$. From the definition (3.27) of the conductivity, we furthermore find the following expression for the Laplace transform $\mathcal{L}(\sigma_0, \Omega)$ of the model conductivity

$$\mathcal{L}(\sigma_0, \Omega) = \frac{e^2}{m} \left(\frac{w^2}{v^2} \frac{1}{\Omega} + \frac{v^2 - w^2}{v^2} \frac{\Omega}{v^2 + \Omega^2} \right)$$

The first order correction $\mathbf{J}_1(t)$ consists of two parts, one that scales with the coupling constant and one that does not. The latter one is given by

$$\mathbf{J}_{1,0}(t) = -\int_{-\infty}^{t} \int e\mathbf{p} \left(\frac{\partial}{\partial t} + e\mathbf{E}(t)\cdot\nabla_{p}\right) f_{0}(\mathbf{p},t')\mathrm{d}\mathbf{p}\mathrm{d}t'.$$
$$= \frac{v^{2} - w^{2}}{v^{2}} \left[\int_{-\infty}^{t} \frac{e^{2}\mathbf{E}(s)}{m}\mathrm{d}s - \int_{-\infty}^{t} \frac{e^{2}\mathbf{E}(s)}{m}\cos v(t-s)\mathrm{d}s\right].$$

The coupling dependent part leads to

$$\mathbf{J}_{1,1}(t) = \frac{e}{m} \int_{-\infty}^{t} \mathrm{d}t' \int_{-\infty}^{t'} \mathrm{d}s$$
$$\sum_{\mathbf{k}} \frac{2 |\gamma(k)|^2}{\hbar} \mathbf{k} \int f_0(\mathbf{p}, s) \left(\begin{array}{c} \left(n_B(\omega_k) + 1 \right) \cos\left(\left(t' - s \right) \left(\frac{\mathbf{k} \cdot \mathbf{p}}{m} + \frac{\hbar k^2}{2m} + \omega_k \right) \right) \\ + n_B(\omega_k) \cos\left(\left(t' - s \right) \left(\frac{\mathbf{k} \cdot \mathbf{p}}{m} + \frac{\hbar k^2}{2m} - \omega_k \right) \right) \end{array} \right) \mathrm{d}\mathbf{p},$$

which within linear response, hence up to O(E), simplifies to

$$\mathbf{J}_{1,1}(t) = -\int_{-\infty}^{t} \mathrm{d}t' \int_{-\infty}^{t'} \mathrm{d}s \chi_{\beta} \left(t'-s\right) \mathbf{J}_{0}(s),$$

with

$$\chi_{\beta}(t) = t \sum_{\mathbf{k}} \frac{2 \left|\gamma\left(k\right)\right|^{2}}{3\hbar} \frac{\mathbf{k}^{2}}{m} \left(\begin{array}{c} \left(n_{B}\left(\omega_{k}\right)+1\right) \sin\left(t\left(\frac{\hbar \mathbf{k}^{2}}{2m}+\omega_{k}\right)\right) \\ +n_{B}\left(\omega_{k}\right) \sin\left(t\left(\frac{\hbar \mathbf{k}^{2}}{2m}-\omega_{k}\right)\right) \end{array} \right) \exp\left(-\frac{\mathbf{k}^{2}}{2m\beta}t^{2}\right).$$

Note that $\lim_{\beta\to\infty} \chi_{\beta}(t) = \chi(t)$, where $\chi(t)$ is the memory function obtained by truncating the equation of motion for the current density, as explained in section 3.4. Consequently the low temperature, linear response, current density up to first order around the Feynman polaron model is

$$\mathbf{J}(t) = \int_{-\infty}^{t} \frac{e^2 \mathbf{E}(s)}{m} \mathrm{d}s - \int_{-\infty}^{t} \mathrm{d}t' \int_{-\infty}^{t'} \mathrm{d}s \chi_{\beta} \left(t' - s\right) \mathbf{J}_0(s).$$
(C.11)

Hence the Laplace transform $\mathcal{L}(\sigma, \Omega)$ of the conductivity reads

$$\mathcal{L}(\sigma,\Omega) = \mathcal{L}(\sigma_0,\Omega) + \mathcal{L}(\sigma_1,\Omega)$$

where the correction to the model conductivity σ_1 is given by

$$\mathcal{L}(\sigma_1,\Omega) = \frac{e^2}{m} \frac{v^2 - w^2}{\Omega(v^2 + \Omega^2)} - \frac{\mathcal{L}(\sigma_0,\Omega)\mathcal{L}(\chi,\Omega)}{\Omega}.$$

A more accurate conductivity can be found using the standard resummation argument

$$\mathcal{L}(\sigma,\Omega) = \mathcal{L}(\sigma_0,\Omega) \left(1 + \frac{\mathcal{L}(\sigma_1,\Omega)}{\mathcal{L}(\sigma_0,\Omega)}\right) \approx \frac{\mathcal{L}(\sigma_0,\Omega)}{1 - \frac{\mathcal{L}(\sigma_1,\Omega)}{\mathcal{L}(\sigma_0,\Omega)}}$$

that is expression (38) in FHIP. Consequently the DC-conductivity for the optical Fröhlich polaron reads

$$\sigma_{DC} = \lim_{\Omega \to 0} \mathcal{L}(\sigma, \Omega) = \frac{w^2}{v^2} \frac{3e^2}{2\alpha m \omega_{LO} n_B(\omega_{LO})}$$

Moreover, since $v^2/w^2 = m^*/m$ [42] we have

$$\sigma_{DC} = \frac{3e^2}{2\alpha m^* \omega_{LO} n_B(\omega_{LO})} \approx \frac{3e^2}{2\alpha m^* \omega_{LO}} e^{\beta \hbar \omega_{LO}}.$$

In agreement with the results obtained in section (3.4). Moreover note that in contrast to FHIP, where the result has a cubic dependence on w/v, the present result depends quadratically on w/v. It is due to this quadratic dependence that the conductivity depends inversely on the effective mass rather then on $(m^*)^{-3/2}$ as in FHIP. Furthermore note that the final resummation is somewhat arbitrary. Allthough it appears logical to resum around the model conductivity one could also argue that the first order correction contains terms that do not explicitly depend on the coupling, i.e. $\mathbf{J}_{1,0}$. These terms only depend on the coupling through the variational parameters v, w. It is clear from expression (C.11) that the model current \mathbf{J}_0 plus this coupling independent pertrubation $\mathbf{J}_{1,0}$ simply equals the free particle response. Resummation around this free particle term is rather natural from the point of expression (C.11). It merely requires to change the model current, on the right hand side of the expression, with the actual current $\mathbf{J}(t)$. Deriving with respect to t furthermore yields

$$\frac{\partial}{\partial t}\mathbf{J}(t) + \int_{-\infty}^{t} \mathbf{J}(s)\chi_{\beta}\left(t-s\right) \mathrm{d}s = \frac{e^{2}\mathbf{E}(s)}{m}.$$
(C.12)

This ought to be compared with (3.47).

Bibliography

- [1] E.P. Wigner, Phys. Rev. 40, 749–759 (1932)
- [2] R. J. Glauber, Phys. Rev. 131, pp. 2766–2788 (1963)
- [3] E. C. G. Sudarshan, Phys. Rev. Lett. **10**, pp. 277–279 (1963)
- [4] C. Gardiner and P. Zoller, *Quantum Noise*, Springer-Verlag, Berlin Heidelberg, third edition, 2004
- [5] S. Deléglise, I. Dotsenko, C. Sayrin, J. Bernu, M. Brune, JM. Raimond, and S. Haroche, Nature 455, 510-514 (2008)
- [6] M. J Steel, M. K. Olsen, L. Plimak, P. D. Drummond, S. M. Tan, M. J. Collett, D. F. Walls, and R.Graham, Phys. Rev. A 58, 4824 (1998)
- [7] A. Polkovnikov, Annals of Physics **325**, 1790–1852 (2010)
- [8] M. Wouters, and V. Savona, Truncated Wigner approximation for nonequilibrium polariton quantum fluids. In D. Sanvitto and V. Timofeev, *Exciton polaritons in microcavities* Heidelberg, Springer, 2012, p. 267-288
- [9] F. Brosens and W. Magnus, phys. stat. sol. B: 246:7, p. 1656-1661 (2009)
- [10] M. Nedjalkov, H. Kosina, P. Schwaha, journal of Computational Electronics 9, 218 223 (2010)
- [11] M. Nedjalkov, D. Vasileska, D.K. Ferry, C. Jacoboni, Ch. Ringhofer, I. Dimov, V. Palankovski, Phys. Rev. B, 74 (2006)
- [12] L. V. Keldysh, Sov. Phys. JETP 20 ,1018 (1965)
- [13] J. Schwinger, J. Math. Phys. 2, 407 (1961)
- [14] L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics, Benjamin New York, 1962
- [15] E.J. Heller, J. Chem. Phys., **65** (4) (1976)
- [16] J.R. Barker and S. Murray, Phys. Lett. A, **93** (6), 271 (1983)
- [17] R.P. Feynman, Reviews of Modern Physics **20**, 367–387 (1948)
- [18] H. Kleinert, Path integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets (5th edition), World Scientific Publishing, 2009, http://klnrt.de/b5
- [19] M. C. Gutzwiller, J. Math. Phys. **12**, 343 (1971).
- [20] J. H. Van Vleck, Proc. Natl. Acad. Sci. U.S.A. 14, 178 (1928).

- [21] M. A. Sepúlveda, S. Tomsovic, and E. J. Heller, Phys. Rev. Lett. 69, 402–405 (1992).
- [22] R. P. Feynman and A. R. Hibbs, Quantum Mechanics and Path Integrals, McGraw-Hill, 1965.
- [23] L. S. Schulman, Techniques and Applications of Path Integration, J. Wiley&Sons, New York, 1981.
- [24] R. P. Feynman and F. L. Vernon, Jr., Annals of physics 24, 118-173 (1963).
- [25] A. O. Caldeira and A. J. Leggett, Physica **121A**, 587–616 (1983)
- [26] Provided the operator has a Taylor expansion in \hat{x}, \hat{p} .
- [27] J. Moyal, Proc. Cambridge Philos. Soc. 45, 99 (1949).
- [28] W.P. Schleich, Quantum Optics in Phase Space, Wiley VCH, Weinheim, 2001.
- [29] R.P. Feynman, The character of physical law, Penguin Books, London, 1992
- [30] N.C. Dias and J.N. Prata, J. Math. Phys. 43, 4602 (2002)
- [31] M. Wilde, *Quantum Information Theory*, Cambridge University Press, 2013.
- [32] D. Sels, F. Brosens and W. Magnus, Physics letters: A **376** (6/7), 809 (2012)
- [33] D. Sels, F. Brosens, and W. Magnus, Physica: A **391**, 78-81 (2012).
- [34] P. Ehrenfest, Zeitschrift für Physik 45, 455–457 (1927).
- [35] M. Suzuki, Physics Letters A **165**, 387–395 (1992).
- [36] Under some debatebly assumptions [25, 37] about the limits in the integral. They can be removed by properly renormalizing the problem from the start.
- [37] M. Rosenau da Costa, A. O. Caldeira, S. M. Dutra, and Jr. H. Westfahl, Phys. Rev. A 61, 22107. (2000).
- [38] J. T. Devreese, J. De Sitter, and M. Goovaerts, Phys. Rev. B 5, 2367 (1972).
- [39] R. P. Feynman, Phys. Rev. **97**, 660 (1955).
- [40] J. T. Devreese, L. F. Lemmens and J. Van Royen, Phys. Rev. B 15, 1212–1214 (1977)
- [41] L. P. Kadanoff, Phys. Rev. **130**, 4 (1963).
- [42] R. Feynman, R. Hellwarth, C. Iddings, and P. Platzman, Phys. Rev. 127, 1004 (1962).
- [43] G. De Filippis, V. Cataudella, A.S. Mishchenko, C.A. Perroni and J.T. Devreese, Phys. Rev. Lett. 96, 136405 (2006).
- [44] S. Klimin and J.T. Devreese, Phys. Rev. B 89, 035201 (2014)
- [45] G. N. A Watson, Treatise on the Theory of Bessel Functions: Chapter XIII, 2nd ed. Cambridge, England: Cambridge University Press, 1966.
- [46] J. Devreese, W. Huybrechts, and L. Lemmens, Phys. Stat.Sol. (b) 48, 77 (1971)

- [47] A.S. Mishchenko, N. Nagaosa, N. V. Prokof'ev, A. Sakamoto, and B. V. Svistunov, Phys. Rev. Lett. 91, 236401 (2003).
- [48] G. De Filippis, V. Cataudella, A. S. Mishchenko, C. A. Perroni, and J. T. Devreese, Phys. Rev. Lett. 96, 136405 (2006)
- [49] J.T. Devreese and S. Klimin, private communication
- [50] V. F. Los', Theor. and Math. Phys. 60, 703 (1984)
- [51] F.M. Peeters, J.T. Devreese, Physica Status Solidi (b) **115**, 539 (1983).
- [52] F.M. Peeters, J.T. Devreese, Solid State Physics, vol. 38, ed. F. Seitz, D. Turnbull, (Academic, New York, 1984), p. 81.
- [53] J. T. Devreese, L. Lemmens, and J. Van Royen, Phys. Rev. B 15, 1212–1214 (1977)
- [54] A. S. Alexandrov and J. T. Devreese, Advances in Polaron Physics, Springer-Verlag Berlin Heidelberg (2010).
- [55] J. T. Devreese, Lectures on Fröhlich Polarons from 3D to 0D, arXiv:1012.4576.
- [56] J.T Devreese and R. Evrard, Phys. Stat. Sol. B 78, 85 (1976).
- [57] J. Hubbard, Phys. Rev. Letters **3**,77 (1959)
- [58] R.L. Stratonovich, Sov. Phys. Dokl. 2, 416 (1958)
- [59] L. I. Plimak, M. K. Olsen, M. Fleischhauer and M. J. Collett, Europhys. Lett. 56, 372 (2001)
- [60] L.I.Plimak, M.Fleischhauer, M.K.Olsen, M.J.Collett, arXiv:cond-mat/0102483
- [61] H. Kleinert, EJTP 8, 57 (2011), http://klnrt.de/391
- [62] R.P. Feynman and H. Kleinert, Phys. Rev. A 34, 5080 (1986)