Quantum field theory

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Part I Introduction

Chapter 1

The big picture: a tourist map of theoretical physics

It's good to keep the big picture in mind, and to start by placing quantum field theory in relation to the other parts of theoretical physics. For that, I give myself the impossible task to review all of the theoretical physics you have seen up till now in the various courses on it.

We start with an overview, a map of the theoretical physics that you have seen in earlier courses – and we situate quantum field theory in that map. The map is roughly split down the middle, with Hamiltonian formulations on the left side, and Lagrangian formulations of the right side.

On the most intuitively clear side of the map, we find classical mechanics. What are "laws of mechanics¹"? To make sense of the world around us, we model it by saying that it can be in a number of different "states of being". For a coin, the states of being can be head or tails. For a classical system of point particles, the state of being can be defined as the list of positions and velocities of these particles. For quantum systems, there is additional structure to the set of possible states, as it turns out to be a vector space. Nevertheless, the character of a law is similar for each of these cases: the laws of mechanics tell us what unique state we'll be in next, given the state we're in now. This is of course a very rough kind of statement, not explaining what "next" means, nor going into the meaning of collapse of wavefunctions upon measurement. However, for classical mechanics it is sufficient to know that by "next" we mean an infinitesimal timestep dt later. Note that in this formulation, laws of mechanics are (forward) deterministic in the sense that for any given state we're in now, there is one unique state that we can be in next.

The split between Hamiltonian and Lagrangian formulations of classical mechanics comes essentially down to a different choice of labeling the states of the system. Both formulations agree that we need to know the (generalized)

¹Check out Feynman's book "the character of physical law" for other insights!

coordinates of all of the particles, q. These can be positions, angles, ... The additional piece of information is the velocity \dot{q} for the Lagrangian formulation², and the momentum p for the Hamiltonian formulation. We can figure out for a given state of being the correct labeling q, \dot{q} for that state, and also the corresponding labeling q, p of that same state. The relation between Hamiltonian and Lagrangian is a Legendre transform, $H(q, p) = p\dot{q} - L(q, \dot{q})$, where the canonical momentum to go from Lagrangian to Hamiltonian is $p = \partial L/\partial \dot{q}$. The "canonical" momentum is not always the same as the "kinematic" momentum $m\dot{q}$.

Classical Mechanics

$$\begin{array}{c} H(q,p) \\ \text{EOM: } \frac{\partial H}{\partial p} = \dot{q}, \frac{\partial H}{\partial q} = \dot{p} \\ \text{conservation law: } \{H,F\} = 0 \end{array} \xrightarrow{p = \frac{\partial L}{\partial \dot{q}}} \begin{array}{c} L(q,\dot{q}) \\ \text{EOM: } \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q} \end{array} \\ & \uparrow \\ S = \int dt \ L(q,\dot{q}) \\ \text{extremal action: } \delta S = 0 \end{array}$$

The dynamics of the system is contained in the Hamiltonian or the Lagrangian. The equation of motion (EOM) specifies the next state, given the current state. In the Hamiltonian formalism we have two first order equations, in the Lagrangian formalism. You've learned to solve these your courses of analytical mechanics, and you learned tricks to tackle the problem when the number of coordinates q_i becomes very large in statistical mechanics. On the side of the Lagrangian formalism, I have added the principle of extremal action. This is an important underlying principle, central to the Lagrangian formulation of quantum mechanics. With each time evolution $q(t), \dot{q}(t)$ of a state, we can associate a score S. Extremizing this score gets you the equations of motion.

Let's move south on the map and go to quantum mechanics. In this second part of the map, we note how a classical theory is quantized.

Quantum Mechanics

operator formalism:		path integral formalism:
$q, p \rightarrow \hat{q}, \hat{p} \& \text{impose } [\hat{q}, \hat{p}] = i\hbar$ EOM: $i\hbar \partial_t \psi(x, t) = \hat{H} \psi$	\longleftrightarrow	$\int \mathcal{D}q \exp\{iS[q(t)]/\hbar\} \text{ gives}$ the transition amplitude

Going down the Hamiltonian path, we quantize by introducing operators, that can act on a state, now described by a wave function = a vector in Hilbert space.

²Note that we can interpret q_t, \dot{q}_t also as knowing q_t now, and q_{t-dt} the previous instant. Both pieces of information are needed to figure out the state in the next instant. So we could say that a law of mechanics determines the state in the next instant from the state in the previous two instances. Rather, we choose to redefine what a state means, and include $\dot{q} = (q_t - q_{t-dt})/dt$ in the labeling.

The equation of motion becomes the Schrödinger equation (although you can reformulate things so you move along with the wave function, and the operators change according to Heisenberg's equation). You've learnt this in your first courses on quantum mechanics. We also have course on Feynman path integrals, showing you that there is another way of doing quantum mechanics, without introducing operators for the position, and keeping the positions and velocities as defining the state of the system. In this formulation you have to take a sum over all possible paths (this sum is denoted by $\int \mathcal{D}q$), each path getting a phase factor $e^{iS/\hbar}$ as a weight. This sum over all paths from an initial state to a final state gives you the quantum mechanical transition amplitude between those states. Both formulations are equivalent: you can derive the Schrödinger equation from the path integral, and obtain the path integral from the Hamiltonian formalism. The path integral formalism nicely links with classical mechanics: only for paths where $\delta S = 0$ the phase factors will add up constructively, showing that the main contribution comes from the classical path.

Classical Field Theory

$\begin{array}{c c} \text{Hamiltonian} \\ \mathcal{H}(\varphi, \pi) \end{array} \xrightarrow{\pi = \frac{\partial L}{\partial(\partial_t \varphi)}}$	Lagrangian density $\mathcal{L}(\varphi, \partial_t \varphi)$ action $S = \int d\mathbf{x} \int dt \ \mathcal{L}(\varphi, \partial_t \varphi)$ extremal action principle $\delta S = 0$
--	---

Sometimes, even in classical physics, it is better to describe the state of the system by a field rather than by the list of coordinates of particles. A field assigns a mathematical object φ to each point in space(time). This object can be simply a scalar (for example the field of temperature in the room, illustrated by an IR camera snapshot), or a more complicated thing, for example a vector (for example the field of wind velocities in a mountain valley). The field $\varphi(\mathbf{x})$ takes on the role of the generalized coordinates $q_i(t)$ where the index *i* (for particle number or degree of freedom) has been replaced by the continuum position vector \mathbf{x} . Again, we will have Hamiltonian and Lagrangian ways of doing classical field theory, depending on whether we describe the current state of being through the field and its canonically conjugated field $\varphi(\mathbf{x}) -$ the Hamiltonian way. You've already had an introductory course on classical field theory, but in order to get our notations in sync I'm going to review this in more detail later in this chapter.

We already went south from classical land to quantum land, but we could also go east, and add *special* relativity to the theory. This changes classical mechanics and equations of motion in that the concept of time has to be refined – now we work in spacetime. In particular, we need to obey covariance and treat space and time on an equal footing, as you saw in your special relativity course.

How about making special relativity compatible with quantum mechanics? Moving east from quantum land, or south from special relativity land, where do we get? Into Quantum field theory! First, let's travel along the Hamiltonian road.

1. Doing this, we first cross the operator mountains: it is clear that the first way that we introduced to quantize the classical theory is not covariant: we promote the spatial position to an operator, but we don't do the same to time. We need a second way to quantize. The solution that has been proposed is *not* to promote also time to an operator (a possibility still being researched), but rather we demote position back to a parameter just like time. It loses its operator character. This forces us to go back to *fields* $\varphi_{\mathbf{x},t}$ where the two are indeed treated on the same footing, and to promote the fields to operators, $\hat{\varphi}_{\mathbf{x},t}$, giving them a special hat to mark the promotion.

2. We're not there yet! We have to sail the Dirac sea next, noting that the number of particles is not fixed! For energies above $2mc^2$ new particleantiparticle pairs can in principle appear. But that is not compatible with the Schrödinger equation, where if you have one particle, you always have 1 particle. So, the quantum fields are operators that can create or annihilate particles.

3. Finally, we come round cape commutator. We finalized quantization by introducing equal-time commutation relations between the operators, and here we have to do the same: $[\hat{q}_j, \hat{p}_{j'}] = i\hbar\delta_{jj'}$ becomes $[\hat{\varphi}_{\mathbf{x},t_0}, \hat{\pi}_{\mathbf{x}',t_0}] = i\hbar\delta(\mathbf{x} - \mathbf{x}')$. And here is a first thing that bothers me about the Hamiltonian road: these are equal-time relations. Quantum mechanics allows you to know position today and momentum tomorrow both with unlimited precision, it is only when you try to know them both at the same time that Heisenberg kicks in. Similary, in the Hamiltonian formulation of quantum field theory, nothing is imposed on $[\hat{\varphi}_{\mathbf{x},t_0}, \hat{\pi}_{\mathbf{x}',t_1}]$. So, whereas the theory treats time and space on the same footing, the commutation relations do not.

You have already encountered the Hamiltonian way of doing quantum field theory, in your course on advanced quantum mechanics. And you can explore it more, and its link to Green's functions for interacting many-body systems, in the course on advanced condensed matter theory. Note that you're free to go from real space to reciprocal space by a Fourier transform:

$$\hat{\varphi}_{\mathbf{x},t} \rightarrow \int d\mathbf{k} \left(e^{-i\mathbf{k}\mathbf{x}} \hat{a}_{\mathbf{k},t} + e^{+i\mathbf{k}\mathbf{x}} \hat{a}_{\mathbf{k},t}^{\dagger} \right)$$
(1.1)

$$\hat{\pi}_{\mathbf{x},t} \rightarrow \int d\mathbf{k} \left(e^{-i\mathbf{k}\mathbf{x}} \hat{a}_{\mathbf{k},t} - e^{+i\mathbf{k}\mathbf{x}} \hat{a}_{\mathbf{k},t}^{\dagger} \right)$$
(1.2)

This links up the fields $\hat{\varphi}, \hat{\pi}$ to the creation and annihilation operators $\hat{a}_{\mathbf{k},t}^{\dagger}, \hat{a}_{\mathbf{k},t}$ for the plane-wave states, that are used in these courses. Doing the transform more carefully brings for free particles terms of the form $\int d\mathbf{k} \left(\hat{a}_{\mathbf{k},t}^{\dagger} \hat{a}_{\mathbf{k},t} + 1/2 \right)$, which include an infinite zero-point contribution. For me, this is another downside to the Hamiltonian road to quantum field theory.

In this course, we're going to follow the Lagrangian road into quantum field theory. We're in the company of authors of good and recent textbooks on quantum field theory. In particular, we will follow the book of A. Zee, "Quantum Field Theory in a Nutshell". Remember that in the Lagrangian road to (nonrelativistic) quantum mechanics we didn't introduce operators so the fields $\varphi_{\mathbf{x},t}$ that describe the system are no longer operators. They are simply the extension of the generalized coordinates q_i whereby the index *i* is replace by a continuum spacetime point \mathbf{x}, t . The dynamics of this field will however still be described by a field Lagrangian $\mathcal{L}(\varphi, \partial_{\mu}\varphi)$, an and associated action $S = \int dx^{\mu} \mathcal{L}(\varphi, \partial_{\mu}\varphi)$ where we integrate over spacetime. Then, Feynman's idea of summing over all possible possibilities becomes a sum over all possible field relazations, each weighed by a phase factor $e^{iS[\varphi_{\mathbf{x},t}]/\hbar}$. No worries if you don't grasp the consequences of this immediately, it takes this whole course to explain...

Quantum Field Theory

What lies beyond? Adding not only special relativity but also general relativity. No-one knows how that works out, but the most promising advances seem to me to lie again along the Lagrangian way. In particular, by again extending the idea of summing over all possible possibilities. Up till now, we had a fixed spacetime theatre on which fields could drape themselves. Listing all possible possibilities comes down to listing all possible values the field can take on this spacetime. To include general relativity, we need to sum over all possible spacetimes as well, and no-one has yet found a conventient way to list and sum all the allowed spacetimes.

Chapter 2

Review: covariant and contravariant tensors

Since many interesting fields have multiple components, and since we want laws of physics that are independent of which coordinate grid you draw over space, our fields will often be tensors as explained below. That is why you need to be proficient in juggling with indices.

Two Rules – Consider a functions $\phi(x^0, x^1, x^2, ..., x^N)$ of N + 1 variables, x^{μ} labeled by $\mu \in \{0, 1, ..., N\}$ in superscript. So it's an upper index and doesn't mean we raise something to some power! These N + 1 variables are considered continuous. We start from two rules that you remember from calculus of functions of multiple variables:

• First rule: the change of ϕ from one point $x = \{x^0, ..., x^N\}$ to the next $x + dx = \{x^0 + dx^0, ..., x^N + dx^N\}$ is

$$d\phi = \sum_{\mu=0}^{N} \frac{\partial \phi}{\partial x^{\mu}} dx^{\mu} = \frac{\partial \phi}{\partial x^{\mu}} dx^{\mu}$$
(2.1)

The last equality shows the "Einstein summation convention" of not writing the summation when we see an index such as μ repeated twice, once as superscript (upper index) and once as subscript (lower index), where the rule is that if an upper index appears in a denominator, it counts as a lower index, and vice versa.

• Second rule: the chain rule. If you go to a different set of coordinates, this means you have N + 1 functions $y^{\lambda}(x)$ (labeled by $\lambda \in \{0, 1, ..., N\}$) that give you the unique set of new coordinates for the same old point. The old coordinates for that point were of course x. The chain rule is then

$$\frac{\partial\phi}{\partial y^{\lambda}} = \sum_{\mu=0}^{N} \frac{\partial\phi}{\partial x^{\mu}} \frac{\partial x^{\mu}}{\partial y^{\lambda}} = \frac{\partial\phi}{\partial x^{\mu}} \frac{\partial x^{\mu}}{\partial y^{\lambda}}$$
(2.2)

The last equality is again showing the Einstein summation convention.

THE ARCHETYPICAL SCALAR – If x and y label the same point, the value $\phi(x) = \phi(y)$ doesn't change. This is the behavior of a scalar. No matter what set of coordinates you whack onto space, ϕ in that point does not change.

THE ARCHETYPICAL CONTRAVARIANT VECTOR – The object to keep in mind when thinking of contravariant vectors is a displacement $dx = \{dx^0, ..., dx^N\}$ such as the one we considered for rule 1. Applying rule number 1 to the functions $y^{\lambda}(x^0, ..., x^N)$ gives

$$dy^{0} = \frac{\partial y^{0}}{\partial x^{\mu}} dx^{\mu}, \quad dy^{1} = \frac{\partial y^{1}}{\partial x^{\mu}} dx^{\mu}, \quad etc.$$

$$\Rightarrow \quad dy^{\lambda} = \frac{\partial y^{\lambda}}{\partial x^{\mu}} dx^{\mu}$$
(2.3)

A contravariant vector is a collection of N + 1 objects v^{μ} , with values in x and y coordinates related by

$$v^{\lambda}(y) = \frac{\partial y^{\lambda}}{\partial x^{\mu}} v^{\mu}(x) \tag{2.4}$$

Here I directly wrote this in Einstein summation convention. You see that the indices that are left over after summing should be the same in left and right hand side of the equation. Both sides have just one upper index λ . You see also that if you switch to a different set of coordinates, the N + 1 components of the vectors will be jumbled up in some linear combination. Linear is good: if you scale up your vectors by a factor 2, they will be scaled up by a factor 2 whatever coordinate grid you slap onto space. You can also add up two vector fields, and the transformed field will still be the sum of the two transformed individual vector fields. In fact, this property is why we call these collections of N + 1 objects vectors in a given point forms a vector space in that point.

CONTRAVARIANT TENSORS – You can construct contravariant tensors by multiplying components of contravariant vectors such as A^{μ} and B^{μ} ,

$$T^{\mu\nu} = A^{\mu}B^{\nu}. \tag{2.5}$$

This is a contravariant tensor of rank 2, meaning it has 2 upper indices. It transforms according to

$$T^{\alpha\beta}(y) = \frac{\partial y^{\alpha}}{\partial x^{\mu}} \frac{\partial y^{\beta}}{\partial x^{\nu}} T^{\mu\nu}(x)$$
(2.6)

which can be checked easily using (2.4). Again the linearity is there. Note that if a tensor is zero in one coordinate grid, it is zero in any coordinate grid. This means that if $T^{\mu\nu} = S^{\mu\nu}$ in one coordinate grid, they are equal in any coordinate grid. That is precisely what we want for our laws of physics: physics should be independent of whatever choice you happen to make for your coordinates – cartesian, cylindrical, spherical,... it all shouldn't matter to the physics, and you can make the choice that makes calculation easiest. In order that laws of physics are independent of the choice of coordinate grid, these laws should be formulated with tensors (both co-and contravariant work)!

THE ARCHETYPICAL COVARIANT VECTOR – The object to keep in mind when thinking of covariant vectors is *the gradient*

$$\partial_{\mu} = \frac{\partial}{\partial x^{\mu}}.$$
(2.7)

The right hand side has a lower index (=an upper index in the denominator), so the left hand side must also have that lower index. From the second rule, we know how the gradient transforms,

$$\frac{\partial}{\partial y^{\lambda}}\phi = \frac{\partial x^{\mu}}{\partial y^{\lambda}}\frac{\partial}{\partial x^{\mu}}\phi.$$
(2.8)

We can generalise this and say that a covariant vector is a set of N + 1 objects v_{μ} with values in x and y coordinates related by

$$v_{\lambda}(y) = \frac{\partial x^{\mu}}{\partial y^{\lambda}} v_{\mu}(x).$$
(2.9)

Note the subtle difference with the prescription for contravariant vectors, expression (2.4). In the street-talk of the dangerous Parisian banlieu, contravariant vectors are called "upper index" vectors, and covariant vectors are called "lower index" vectors, for obvious reasons.

MORE TENSORS – Again you can make covariant tensors of higher rank by multiplying covariant vectors

$$T_{\mu\nu} = A_{\mu}B_{\nu}.\tag{2.10}$$

This rank-2 example transforms according to

$$T_{\alpha\beta}(y) = \frac{\partial x^{\mu}}{\partial y^{\alpha}} \frac{\partial x^{\nu}}{\partial y^{\beta}} T_{\mu\nu}(x).$$
(2.11)

You can also make tensors of mixed nature, with both upper and lower indices,

$$T^{\mu.}_{.\nu} = A^{\mu}B_{\nu}$$

$$\Rightarrow T^{\alpha.}_{.\beta}(y) = \frac{\partial y^{\alpha}}{\partial x^{\mu}}\frac{\partial x^{\nu}}{\partial y^{\beta}}T^{\mu.}_{.\nu}(x)$$
(2.12)

Check out the Einstein summation and the left hand side - right hand side correspondence in this one! You can "trace out" an index here: $T^{\mu}_{.\mu}$ (with the

Einstein summation convention) is just a scalar. This is called "contracting a tensor" and reduces its rank by 2. For example

$$T_{\alpha\beta} = T^{\dots\mu}_{\alpha\mu,\beta} \tag{2.13}$$

Now you also see why we put the dots: to indicate that it is the third index which is the upper index. It's not needed, you can usually figure out what you have, but sometimes when there are some symmetries in index swapping this notation is useful.

THE METRIC TENSOR – We don't venture into spacetime yet, and look at a nice flat piece of space. We can slap cartesian coordinates on that. Then the distance between two (infinitesimally close) points related by a displacement dx^{μ} is given by the Pythagorean rule

$$ds^{2} = (dx^{0})^{2} + (dx^{1})^{2} + \dots + (dx^{N})^{2}$$
(2.14)

OK, now the "2"s outside the bracket are indeed squares. We could write this as

$$ds^2 = dx^\mu \delta_{\mu\nu} dx^\nu \tag{2.15}$$

with $\delta_{\mu\nu}$ the Kronecker delta (=1 when $\mu = \nu$, and zero otherwise). It has lower indices, so we get summations over both μ and ν . If you switch from cartesian coordinates to something else, you get from rule #1:

$$ds^{2} = dy^{\alpha} \underbrace{\frac{\partial x^{\mu}}{\partial y^{\alpha}} \delta_{\mu\nu} \frac{\partial x^{\nu}}{\partial y^{\beta}}}_{q_{\alpha\beta}} dy^{\beta} = dy^{\alpha} g_{\alpha\beta} dy^{\beta}$$
(2.16)

The object $g_{\alpha\beta}$ clearly transforms like a covariant tensor of rank 2. It is called the *metric tensor*. It is present not only in flat space (with or without curvilinear coordinates), but is also used to define infinitesimal distances in curved space. In fact, if there exists a coordinate transform that can bring $g_{\alpha\beta}$ back to $\delta_{\alpha\beta}$ then we say that space is flat – the definition of curved space is that such a coordinate transform cannot be found. So you cannot see at first glance from $g_{\alpha\beta}$ whether space is flat or curved, it may just be that you use silly coordinates on a perfectly flat table. You'd have to calculate the curvature tensor to check that, or do some parallel transport, the realm of general relativity.

PUMPING INDICES – The metric is symmetric, $g_{\mu\nu} = g_{\nu\mu}$, and has an inverse:

$$g^{\mu\alpha}g_{\alpha\nu} = \delta^{\mu}_{.\nu} \tag{2.17}$$

where $\delta^{\mu}_{,\nu}$ is again a Kronecker delta, equal to one when $\mu = \nu$ and zero otherwise. This can be used to set up a relation between covariant and contravariant tensors. Indeed, with any contravariant vector A^{μ} you can associate a covariant one through

$$A_{\nu} = A^{\mu}g_{\mu\nu} \tag{2.18}$$

The metric tensor is used to "pump" indices up or down in general

$$T^{\mu}_{,\nu} = g^{\mu\alpha} T_{\alpha\nu} \tag{2.19}$$

This also allows you to contract tensors that are compeletely co- or covariant:

$$T_{\alpha\beta} = T_{\alpha\mu\nu\beta}g^{\mu\nu} = T^{.\nu..}_{\alpha.\nu\beta} = T^{..\mu..}_{\alpha\mu.\beta}.$$
 (2.20)

Chapter 3

Review: Group Theory

Symmetry will be an important aspect of setting up field theories. Symmetries are based on invariance with respect to transformations. Transformations form mathematical objects called groups, and to understand the important role of symmetry in field theory you need to be familiar with at least the basics of group theory.

DEFINITION OF A GROUP – Consider a set \mathcal{T} of elements such as transformations¹ – we can have a finite set $\mathcal{T} = \{T_1, T_2, \ldots, T_N\}$, a denumerable set $\mathcal{T} = \{T_1, T_2, T_3, \ldots\}$ or a nondenumerable set $\mathcal{T} = \{T_\theta\}_{\theta}$ indexed by one or more continuous group parameters θ . This set is equipped with a composition rule, that enables you to construct a new transformation T_c by applying two transformations T_bT_a in succession. The first property that should be fulfilled in order for the set with its composition rule to be called a group is the closure property. This states that all the transformations that we can construct by composing existing ones, are already part of the set, so:

Closure:
$$\forall T_a, T_b \in \mathcal{T} : T_b T_a \in \mathcal{T}$$
 (3.1)

Apart from that, three other axioms must be satisfied:

Associative : $\forall T_a, T_b, T_c \in \mathcal{T} : T_c (T_b T_a) = (T_c T_b) T_a$ (3.2) Neutral element : $\exists I \in \mathcal{T} : \forall T_a \in \mathcal{T} : IT_a = T_a I = T_a$ (3.3) Symmetric element : $\forall T_a \in \mathcal{T} : \exists T_b \in \mathcal{T} : T_a T_b = T_b T_a = I$ (3.4)

The neutral element is often called the identity. For transformation groups it is the transformation that maps all elements of X onto itself.

¹Here we indeed focus on *transformation groups* the elements of which act on a certain space X preserving its inherent structure. Permutation groups ans matrix groups are special cases. In the case of permutation groups, X is a set; for matrix groups, X is a vector space. Symmetry groups are another special case: they consists of all transformations that preserve a more specific structure - they could preserve a Lagrangian, or preserve orthogonality, or map a triangle onto itself,...

If moreover the order in which the elements are combined doesn't matter, $T_aT_b = T_bT_a$ for all $T_a, T_b \in \mathcal{T}$, the group is called abelian or commutative. In case the order does matter, it is non-abelian or non-commutative.

REPRESENTATION OF A GROUP – Formally, a group representation is a "mapping of all group elements into linear operators that preserve the composition rule". In my mind, I think of linking each element $T_a, T_b, T_c, ...$ of the group to a matrix $M_a, M_b, M_c, ...$ such that (1)

$$T_c = T_a T_b \Rightarrow M_c = M_a \cdot M_b \tag{3.5}$$

and (2) the identity element or neutral element is mapped onto the identity matrix. Here \cdot indicates matrix multiplication. There are usually many different ways to choose good matrices, and thus many different representation. If all the matrices M_a can be diagonalized or block-diagonalized $P^{-1}M_aP$ by the same unitary transformation P we say that the representation is *decomposable*. The rank of the matrices is the *dimension* of the representation. Loosely speaking, if you have a representation but you can find matrices of smaller rank that still form a good representation, then we call this a "*reducible*" representation. The opposite is an *irreducible* representation.

LIE GROUP – Discrete groups have a denumerable or finite number of elements, but most transformation groups depend on continuous parameters. We define a *Lie group* as a group

- that depends on a (finite) set of continuous parameters θ_i , such that the identity element corresponds with all $\theta_i = 0$, and
- for which the derivatives of the group elements with respect to the parameters exist.

The second condition can be interpreted as follows: if you have a representation $M(T_{\theta})$ of the group, then these matrices will depend on $\theta = \{\theta_1, \theta_2, ..\}$. If you can take derivatives of all matrix elements with respect to the θ_i , then it's OK. This implies that you can think of "large" transformations as a succession of many "small" transformations. For example, consider rotations over an angle θ in the xy-plane. These form a continuous group with 1 group parameter, θ . They can be represented by 2×2 matrices:

$$R_{\theta} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

such that $\theta = 0$ indeed gives us the identity matrix. Moreover,

$$\frac{dR_{\theta}}{d\theta} = \begin{pmatrix} -\sin\theta & \cos\theta \\ -\cos\theta & -\sin\theta \end{pmatrix}$$
(3.6)

exists (i.e. is nowhere singular). So, this is a Lie group. You can also think of rotations over a large angle as a succession of many rotations over a small angle.

GENERATORS OF THE GROUP – If we're going to think of every Lie group element as a succession of infinitesimal transformations, these transformations with θ infinitesimal take a special place in the theory. For a Lie group with parameters $\theta = \{\theta_1, \theta_2, ...\}$ and representation M_{θ} , we can expand around the origin

$$M_{\theta} = \underbrace{M_{0}}_{\text{unit matrix}} + \sum_{j} \underbrace{\frac{\partial M}{\partial \theta_{j}}}_{\text{generators}} \theta_{j} + \dots$$
(3.7)

There are as many generators of the group as there are continuous parameters. The generators are defined with an additional factor -i, so by definition

$$X_j = -i \left. \frac{\partial M}{\partial \theta_j} \right|_{\theta \to 0} \tag{3.8}$$

is the j-th generator of the group, and we can write

$$M_{\theta} = I + i \sum_{j} X_{j} \theta_{j} + \mathcal{O}(\theta^{2}).$$
(3.9)

Now the idea of splitting a large-parameter element up in a succession of infinitesimalparameter ones pays of, since we can write for *any* element:

$$M_{\theta} = \lim_{N \to \infty} \left(M_{\theta/N} \right)^N = \lim_{N \to \infty} \left(1 + iX \frac{\theta}{N} \right)^N = \exp\left\{ iX\theta \right\}$$
(3.10)

The first equality expresses our idea of many small steps, the second equality exploits the fact that the step is small. So, once you know the generators of the group, it is easy to write the representation of an element for any $\theta = \theta_1, \theta_2, ...$ value:

$$M_{\theta} = \exp\left\{i\sum_{j} X_{j}\theta_{j}\right\}$$
(3.11)

The factor "i" is handy: if the matrix X is hermitean, the matrix M_{θ} is unitary! We'll discuss generators for a bunch of relevant transformations in a later chapter, but for here let's go back to the example of 2D rotations. The generator in the representation that we have used is

$$X = -i \left. \frac{dR_{\theta}}{d\theta} \right|_{\theta \to 0} = i \lim_{\theta \to 0} \left(\begin{array}{cc} \sin \theta & -\cos \theta \\ \cos \theta & \sin \theta \end{array} \right) = \left(\begin{array}{cc} 0 & -i \\ i & 0 \end{array} \right)$$
(3.12)

So,

$$X^{2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$
(3.13)

and hence $X^{2n} = I$, $X^{2n+1} = X$. Then splitting up the sum

$$R_{\theta} = \exp\left\{iX\theta\right\} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(i\theta\right)^n X^n \tag{3.14}$$

into even and odd subsums gives

$$R_{\theta} = \exp\left\{iX\theta\right\} = \sum_{n=0}^{\infty} \frac{(-1)^n \,\theta^{2n}}{(2n)!} I + \sum_{n=0}^{\infty} \frac{(-1)^n \,\theta^{2n+1}}{(2n+1)!} iX \tag{3.15}$$

This is

$$R_{\theta} = \sum_{n=0}^{\infty} \frac{(-1)^n \,\theta^{2n}}{(2n)!} \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix} + \sum_{n=0}^{\infty} \frac{(-1)^n \,\theta^{2n+1}}{(2n+1)!} \begin{pmatrix} 0 & 1\\ -1 & 0 \end{pmatrix}$$
(3.16)

The first sum is the series representations of $\cos(\theta)$, and the second is the series representation of $\sin(\theta)$, so

$$R_{\theta} = \cos(\theta) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sin(\theta) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}.$$
 (3.17)

It works! The rule $R_{\theta} = \exp\{iX\theta\}$ brings us back to the correct matrix for any rotation in our example.

LIE ALGEBRA – In our previous example, we seemed to be quite lucky that products of I and X stayed "amongst friends", i.e. any product was still \in $\{I, X\}$. This is no coincidence. If we have many generators $X_1, X_2, ..., X_N$ we could look at the set of matrices $\{I, X_1, ..., X_N\}$ and find that if you multiply two, you'll always get some linear combination of the others. Considering addition and scalar multiplication of matrices (the stuff you need for linear combinations) you can make a vector space, but if you add the matrix multiplication to this, you get a structure known as an "algebra". Using $\{I, X_1, ..., X_N\}$ as the basis for this algebra gives you the *Lie algebra* of the group.

In general, the structure of this Lie algebra is fixed by the commutation relations between the generators, and we have

$$[X_j, X_k] = i f_{jk\ell} X_\ell$$

where the constants $f_{jk\ell}$ are called the *structure constants* of the group. A well known example are the Pauli matrices – the generators of the group of all unitary 2×2 matrices with determinant 1, called SU(2), or the angular momenta (the generators of the group of rotations). Often the relation of the different generators to eachother can be clarified by seeing them as elements of a tensor (the angular momenta can be collected into an antisymmetric rank 2 covariant tensor as we will see).

Chapter 4

Review: special relativity

Quantum field theory is the marriage between special relativity and quantum theory. So it is obvious you ought to know special relativity to follow this course.

Distance in spacetime

In special relativity, events take place in points x in spacetime, characterized by four coordinates x^{μ} ,

$$x = \{x^0, x^1, x^2, x^3\}$$

In flat space we can use cartesian coordinates

$$x = \{ct, x, y, z\} = \{ct, \vec{x}\}$$

There will be ambiguity in our notations: x sometimes means the point in spacetime, and sometimes the x-cartesian coordinate. Hopefully it will be clear from the context. Distances in spacetime differ from the Euclidean distances, in that the metric for flat spacetime is determined by

$$ds^{2} = (dx^{0})^{2} - (dx^{1})^{2} - (dx^{2})^{2} - (dx^{3})^{2}$$

$$(4.1)$$

More ambiguity: the "2" outside the bracket is a power. The overal sign of this distance is the convention that I follow – the books don't agree. But I like to use this sign for the "distance" in order to think of it as eigen-time measure by a clock at the point x. For tensor calculus we know that we should write this as

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu, \qquad (4.2)$$

cf. expression (2.16). Our flat spacetime metric is

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1 \end{pmatrix} = g^{\mu\nu}$$
(4.3)

In flat spacetime, we can always find "cartesian" coordinates that bring the metric to this form. We won't look at curved spacetime (a lot) since quantum field theory fails to describe gravity anyway.

We're often going to use *cartesian coordinates in Minkowski space*. This leads to possible confusion in notations. The following list is an attempt to resolve this ambiguity:

since
$$x^0, x^1, x^2, x^3$$
 corresponds to ct, x, y, z
then x_0, x_1, x_2, x_3 corresponds to $ct, -x, -y, -z$
and $\partial_0, \partial_1, \partial_2, \partial_3$ corresponds to $\frac{1}{c} \frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}$
and $\partial^0, \partial^1, \partial^2, \partial^3$ corresponds to $\frac{1}{c} \frac{\partial}{\partial t}, -\frac{\partial}{\partial x}, -\frac{\partial}{\partial y}, -\frac{\partial}{\partial z}$

With $\partial_0, \partial_1, \partial_2, \partial_3$ we mean $\frac{\partial}{\partial x^0}, \frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2}, \frac{\partial}{\partial x^3}$, and with $\partial^0, \partial^1, \partial^2, \partial^3$ here we mean $\frac{\partial}{\partial x_0}, \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}$. So, in particular we have

$$\partial_{\mu}\partial^{\mu}f = \partial^{\mu}\partial_{\mu}f = \left(\frac{1}{c^{2}}\frac{\partial^{2}}{\partial t^{2}} - \frac{\partial^{2}}{\partial x^{2}} - \frac{\partial^{2}}{\partial y^{2}} - \frac{\partial^{2}}{\partial z^{2}}\right)f$$
(4.4)

and

$$x_{\mu}x^{\mu} = x^{\mu}x_{\mu} = (ct)^2 - x^2 - y^2 - z^2$$
(4.5)

with minus signs, but

$$x^{\mu}\partial_{\mu}f = x_{\mu}\partial^{\mu}f = \left(t\frac{\partial}{\partial t} + x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z}\right)f$$
(4.6)

without. Finally, note that in first quantization we have

$$\left(\hat{H}, \hat{\vec{p}}\right) \equiv \left(i\hbar\frac{\partial}{\partial t}, -i\hbar\vec{\nabla}\right) = i\hbar\partial^{\mu}$$
(4.7)

where we replace the *contravariant* components. So, we'll get an equivalence $p^{\mu} \longleftrightarrow i\hbar\partial^{\mu}$ and $p_{\mu} \longleftrightarrow i\hbar\partial_{\mu}$, from which it follows that plane waves (eigenfunction of the momentum operator) are $e^{ip_{\mu}x^{\mu}/\hbar}$. With $p^{\mu}/\hbar = k^{\mu} = (\omega, \vec{k})$ these plane wave solutions are $e^{i\omega t - i\vec{k}\vec{x}}$. We'll use those to define the Fourier transform of functions,

$$f(k) = \int d^4x \ f(x)e^{+ik_{\mu}x^{\mu}}$$
(4.8)

$$f(x) = \int \frac{d^4k}{(2\pi)^4} f(k) e^{-ik_{\mu}x^{\mu}}$$
(4.9)

from which we get the Fourier representation of the delta function,

$$\delta(x-y) = \int \frac{d^4k}{(2\pi)^4} e^{ik_\mu (x^\mu - y^\mu)} = \delta(y-x)$$
(4.10)

Lorentz-invariance

Why does special relativity require such a weird expression for the distance $d\tau$? To understand that, we need to introduce a coordinate transform called the Lorentz-boost. A Lorentz-boost with velocity \vec{v} along the x-axis is a transformation determined by

$$ct' = \frac{1}{\sqrt{1 - \vec{v}^2/c^2}} [ct - (|\vec{v}|/c)x]$$

$$x' = \frac{1}{\sqrt{1 - \vec{v}^2/c^2}} [x - (|\vec{v}|/c)(ct)]$$

$$y' = y$$

$$z' = z$$

This brings us from the old coordinates $\{ct, x, y, z\}$ to a new set of coordinates $\{ct', x', y', z'\}$ that would be used by an observer moving at constant velocity \vec{v} . Sets of coordinates are often also called "frames of reference" in special relativity. The arrow on top of \vec{v} reminds us that this is a 3-vector in space, and not a 4-vector in spacetime. So \vec{v} is the velocity that you are familiar with from classical Newtonian mechanics. In tensor notation, we can write this coordinate transform as

$$(x')^{\mu} = L^{\mu}_{,\nu} x^{\nu} \tag{4.11}$$

with

$$L^{\mu.}_{,\nu} = \frac{\partial (x')^{\mu}}{\partial x^{\nu}} = \begin{pmatrix} \frac{1}{\sqrt{1 - \vec{v}^2/c^2}} & -\frac{|\vec{v}|/c}{\sqrt{1 - \vec{v}^2/c^2}} & 0 & 0\\ -\frac{|\vec{v}|/c}{\sqrt{1 - \vec{v}^2/c^2}} & \frac{1}{\sqrt{1 - \vec{v}^2/c^2}} & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1 \end{pmatrix}$$
(4.12)

with the rapidity $\vartheta = \operatorname{arctanh}(\left|\vec{v}\right|/c)$ this can be written as

$$L^{\mu.}_{,\nu} = \begin{pmatrix} \cosh(\vartheta) & -\sinh(\vartheta) & 0 & 0\\ -\sinh(\vartheta) & \cosh(\vartheta) & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1 \end{pmatrix}$$
(4.13)

A contravariant 4-vector A^{μ} transforms under the Lorentz transformation as

$$L^{\mu.}_{,\nu}A^{\nu}(x) = A^{\mu}(x') \tag{4.14}$$

This also holds for the archetypical contravariant vector dx^{μ} so that

$$dx^{\mu}dx^{\nu} \to L^{\mu}_{.\alpha}L^{\nu}_{.\beta}dx^{\alpha}dx^{\beta}$$
(4.15)

Then ds^2 is unaffected by the Lorentz boost if

$$g_{\alpha\beta} = g_{\mu\nu}(x) L^{\mu.}_{.\alpha} L^{\nu.}_{.\beta} \tag{4.16}$$

 since

$$ds^{2} = g_{\mu\nu}(x)dx^{\mu}dx^{\nu} \rightarrow \underbrace{g_{\mu\nu}(x)L^{\mu}_{,\alpha}L^{\nu}_{,\beta}}_{g_{\alpha\beta}}dx^{\alpha}dx^{\beta}$$
(4.17)

This is true for any \vec{v} only if we have the minus signs in the metric (again, up to an overall sign).

The set of different Lorentz-boosts (for all different \vec{v} 's) together with the rotations of spatial coordinates form a Lie group. The three components of the velocity are continuous parameters of the group, and $\vec{v} = 0$ obviously gives the identity transform. The set of different frames of reference that we can obtain by Lorentz boosts are called the "Lorentz frames of reference".

This coordinate transform takes a central role because the Maxwell equations are invariant with respect to them. The Maxwell equations have the same for, irrespective of which Lorentz frame of reference you use. Einstein generalized this to all of physics: he requires that any law of physics should be Lorentz invariant. This is a bold move, requiring space and time to be more closely knitted together.

Eigen-time and relativistic momentum

The eigen-time is another important concept in special relativity. Take a particle or an observer moving at constant velocity \vec{v} . You can attach a Lorentz frame of reference to this particle, so that the spatial origin of the frame of reference moves along with the particle. We call this the frame of reference of the particle. The time elapsed in this frame of reference is the eigen-time τ . The particle is always at the spatial origin of its own frame of reference, so

$$\{(x')^0, (x')^1, (x')^2, (x')^3\} = \{\tau, 0, 0, 0\}$$
(4.18)

We can imagine that the particle has a clock, for example a pulse of light bouncing between two mirrors intricately built into a wristwatch. Each time the pulse bounces of a mirror the clock advances one tick. By definition the eigen-time is Lorentz-invariant: all observers will agree on the time elapsed on that specific clock, even though it does not match the time elapsed on their own clock.

Any infinitesimal distance ds is invariant, and in the particles own frame of reference we have $ds = cd\tau$. With this invariant or scalar, we can construct a new contravariant vector from an old one. Let's take the archetypical contravariant vector

$$dx^{\mu} = \{cdt, dx, dy, dz\}$$

$$(4.19)$$

and divide it by $d\tau$:

$$u^{\mu} = \frac{dx^{\mu}}{d\tau} = \{c\frac{dt}{d\tau}, \frac{dx}{d\tau}, \frac{dy}{d\tau}, \frac{dz}{d\tau}\}$$
(4.20)

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This transforms indeed like a four-vector $(u')^{\mu} = L^{\mu}_{,\nu} u^{\nu}$. And since

$$\sqrt{1 - \vec{v}^2/c^2}dt = d\tau \tag{4.21}$$

we get

$$u^{\mu} = \frac{dx^{\mu}}{d\tau} = \frac{1}{\sqrt{1 - \vec{v}^2/c^2}} \frac{dx^{\mu}}{dt} = \frac{1}{\sqrt{1 - \vec{v}^2/c^2}} \{c, \vec{v}_x, \vec{v}_y, \vec{v}_z\}$$
(4.22)

where $\vec{v}_x = dx/dt$ is the x-component of the Newtonian spatial velocity. The four-vector u^{μ} is the velocity-fourvector. Another invariant is the rest mass m of the particle, so we can construct yet another contravariant vector

$$p^{\mu} = mu^{\mu} = \left\{ \frac{mc}{\sqrt{1 - \vec{v}^2/c^2}}, \frac{m\vec{v}_x}{\sqrt{1 - \vec{v}^2/c^2}}, \frac{m\vec{v}_y}{\sqrt{1 - \vec{v}^2/c^2}}, \frac{m\vec{v}_z}{\sqrt{1 - \vec{v}^2/c^2}} \right\}$$
(4.23)

This is the (kinematic) *momentum-fourvector*. We can rewrite it in a more Newtonian notation as

$$p^{\mu} = \left\{ \frac{E}{c}, \vec{p}_x, \vec{p}_y, \vec{p}_z \right\}$$

$$(4.24)$$

The natural occurence of the momentum is as a covariant rather than a contravariant vector (in that covariant is a bit like the reciprocal space in crystallography; in that space the wave number lives, which combines with position to form a dimensionless scalar). So for completeness, we pump the index down with the metric:

$$p_{\mu} = g_{\mu\nu} p^{\nu} = \left\{ -\frac{E}{c}, \vec{p}_x, \vec{p}_y, \vec{p}_z \right\}$$
(4.25)

This new four-vector allows to make another Lorentz invariant. Indeed, $p^2 = p^{\mu}p_{\mu}$ is a Lorentz-invariant. All observers agree on

$$p^{\mu}g_{\mu\nu}p^{\nu} = -\frac{(mc)^2}{1 - \vec{v}^2/c^2} + \frac{(m\vec{v}_x)^2 + (m\vec{v}_y)^2 + (m\vec{v}_z)^2}{1 - \vec{v}^2/c^2}$$
(4.26)

and since $\vec{v}_x^2 + \vec{v}_y^2 + \vec{v}_z^2 = \vec{v}^2$ we get

$$p^{2} = -m^{2} \frac{c^{2} - \vec{v}^{2}}{1 - \vec{v}^{2}/c^{2}} = -(mc)^{2}$$
(4.27)

On the other hand, we find from (4.24) that this is equal to

$$p^2 = -\left(\frac{E}{c}\right)^2 + \vec{p}^2 \tag{4.28}$$

from which we derive

$$(mc)^{2} = (E/c)^{2} - \vec{p}^{2} \Leftrightarrow E^{2} = (mc^{2})^{2} + (\vec{p}c)^{2}$$
(4.29)

This is the adult version of the baby-slogan $E = mc^2$. Babies generally have negligible three-momentum \vec{p} anyway. Even though energy E and three-momentum \vec{p} can be different for different observers, the length of the four-momentum will be the same for all observers, namely $-(mc)^2$ (so it's negative in our metric).

We can go on. The four-momentum can be combined with the scalar $d\tau$ to define a four-force:

$$K^{\mu} = \frac{dp^{\mu}}{d\tau} \tag{4.30}$$

Again we can switch from the particle's frame of reference to time in our own frame of reference:

$$K^{\mu} = \frac{1}{\sqrt{1 - \vec{v}^2/c^2}} \frac{dp^{\mu}}{dt} = \frac{1}{\sqrt{1 - \vec{v}^2/c^2}} \left\{ \frac{1}{c} \frac{dE}{dt}, \vec{F}_x, \vec{F}_y, \vec{F}_z \right\}$$
(4.31)

where $\vec{F} = d\vec{p}/dt$ is the Newtonian force vector in space. The first component is dE/dt, and just as in Newtonian physics it is given by $\vec{F} \cdot \vec{v}$. Indeed, $p^{\mu}p_{\mu}$ is a constant, from which we find

$$0 = \frac{d(p^{\mu}p_{\mu})}{d\tau} = 2\frac{dp^{\mu}}{d\tau}p_{\mu} \Rightarrow K^{\mu}p_{\mu} = 0$$

and in the Minkowski metric this means

$$\frac{1}{1 - \vec{v}^2/c^2} \left[-\left(\frac{1}{c}\frac{dE}{dt}\right)mc + \vec{F} \cdot (m\vec{v}) \right] = 0$$
$$\Leftrightarrow \frac{dE}{dt} = \vec{F} \cdot \vec{v}$$
(4.32)

Relativistic energy

Like Einstein suggested, we demand that the action functional is Lorentz invariant. For a short piece of world line the simplest Lorentz invariant is $ds = cd\tau$, with $d\tau$ de eigen-time. For the entire trajectory we can add up these piece and propose the world line length for the action:

$$\mathcal{S} := -mc \int ds = -mc^2 \int d\tau \tag{4.33}$$

The action functional has units of energy times time, so to get this right we multiplied our proposal by the other constant available: the particle's rest mass. This action measues the number of ticks on the particle's own clock, between the starting point and the final point along its world-line path in Minkowski space. This will be something all observers agree about. On the clock of an observer who claims that the particle moves with a 3-velocity \vec{v} , a lapse $d\tau$ corresponds to

$$\sqrt{1 - \vec{v}^2 / c^2} dt = d\tau, \tag{4.34}$$

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the famous time dilatation. For the observer the clock of the moving particle appears to tick more slowly than his own clock $d\tau < dt$. So, if this observer wants to calculate S using the values measures his own frame of reference, he will find

$$S = -mc^2 \int \sqrt{1 - \vec{v}^2/c^2} dt$$
 (4.35)

$$\rightarrow \quad L = -mc^2 \sqrt{1 - \vec{v}^2/c^2} \tag{4.36}$$

For small times, this agrees with the usual Lagrangian for a particle moving with velocity \vec{v} ,

$$\lim_{v < < c} L = -mc^2 + \frac{1}{2}m\vec{v}^2 + \mathcal{O}\left[(v/c)^4\right], \qquad (4.37)$$

where a constant rest energy term has been subtracted – constants don't affect the equation of motion. Now it is also clear why we chose the minus sign in (4.33): to get the good Newtonian limit. Nu is het ook duidelijk waarom we een minteken kiezen in de definitie van de relativisitische actie van een vrij deeltje; om het juiste teken voor de klassieke Lagrangiaan te herbekomen.

The canonical momentum that we derive from this Lagrangian is

$$\vec{p} := \frac{\partial L}{\partial \vec{v}}$$

$$\rightarrow \vec{p} = \frac{m\vec{v}}{\sqrt{1 - \vec{v}^2/c^2}}$$
(4.38)

Here it matches the kinematic momentum that we defined earlier. The Hamiltonian then becomes

$$H := \vec{p} \cdot \vec{v} - L \tag{4.39}$$

Substituting the expressions for \vec{p} and \mathcal{L} gives

$$H = \frac{m\vec{v}^2}{\sqrt{1 - \vec{v}^2/c^2}} + mc^2\sqrt{1 - \vec{v}^2/c^2} = \frac{mc^2}{\sqrt{1 - \vec{v}^2/c^2}}$$
(4.40)

Or, if you want to write this as a function of \vec{p} ,

$$H = mc^2 \sqrt{1 + \frac{\vec{p}^2}{(mc)^2}} = \sqrt{m^2 c^4 + \vec{p}^2 c^2}$$
(4.41)

This is the well-known formula

$$E^2 = (mc^2)^2 + (\vec{p}c)^2$$

. We see from it that relativistic effects will start to matter when $|\vec{p}|/mc$ becomes compareable to 1. In quantum mechanics, $\vec{p} = \hbar \vec{k}$, so that we can say that in quantum mechanics, relativistic effects become important at distances compareable with $\lambda_C = \hbar/(mc)$, the Compton wavelength. When wave functions vary over distances compareable to the Compton wave length, you have to work relativistically and use quantum field theory!

Final remarks and relativistic strings

OK, this may not be something you just need to review a bit. But it is fun.

The action functional, written as the world line length $\int ds$, could still be used in curves space, where the metric is very different since it has to satisfy the Einstein equations of general relativity. The link between world line length and metric is again

$$ds^{2} = g_{\mu\nu}dx^{\mu}dx^{\nu} = g_{\mu\nu}\frac{dx^{\mu}}{d\tau}\frac{dx^{\nu}}{d\tau}(d\tau)^{2}$$
(4.42)

so that

$$S = -mc \int ds = -mc \int \sqrt{g_{\mu\nu} \frac{dx^{\mu}}{d\tau} \frac{dx^{\nu}}{d\tau}} d\tau \qquad (4.43)$$

If you plug in the Minkowski metric and (4.22), you retrieve expression (4.35) for flat space.

Not only can you keep using this expression in general relativity, but it can be used to try and marry the theory with quantum mechanics by using this action functional in a path integral. This remains true in string theory. Now we have strings, tracing out world tubes rather than world lines. The string theory action is proportional to the surface of this world tube – a straightforward realization of what we have here. That surface is also a Lorentz-invariant!

As a FINAL FINAL REMARK ON THIS TOPIC – Do you also get very tired of dragging all these factors 'c' around just because some French guy decided to measure time in seconds and distances in meters? Let's adapt our unit of time so we have the same units for ct as for x, y, z. This comes down to setting c = 1, and choosing as a unit of time the time it takes for light to cross a unit of length, in vacuum.

Part II

Classical Lagrangian field theory

Chapter 5

Fields and transformations

5.1 Fields as a continuum limit

Typical problems in classical field theory involve finding the shape of a circular membrane after it was hit, or the electromagnetic field modes of some cavity, or the velocities and densities of a fluid flowing through a pipe. We want to find the classical result for the field of displacements, potential, velocity,... and we know it obeys a certain field equation. This could be the wave equation, or the diffusion equation, or the Helmholtz equation. How do these concepts relate to analytical mechanics of mass points as we take the continuum limit? Let us investigate this with a concrete example.

Consider a simple classical model of N mass points with mass m, labeled by an index $j \in \{1, 2, ..., N\}$, and connected by springs. We'll simplify the picture even more by saying that the points can only move up or down, their positions on the x-axis is fixed, Mass point j is located at $x = \varepsilon j$. The height will be denoted by q_j . This looks a bit like a 1D mattress or, better, a violin string suspended between bridge (x = 0) and peg (x = N), as in the following picture:



Note that the x just label which mass we talk about, but it is not a degree of freedom! Only the q_j 's are the degrees of freedom, our generalized coordinates.

We could just as well have labeled them q_x and we will do so later. You can already surmise that we'll add more and more mass points and shrink the gap ε down to zero to get to fields. However, if we keep adding more closely spaced mass points, the mass of our springy string will go to infinity and we need to avoid that. What we want is that a given segment of string has a given mass. To ensure this we will have to shrink the mass of the particles as we add more and more: the mass has to shrink proportionally to ε . So let's take $m = \mu \varepsilon$ with μ the mass per unit string length.

So what would be the action of this system, literally thinking of this as a collection of mass points and springs? The kinetic energy will be

$$T = \frac{1}{2} \sum_{j} m \dot{q}_{j}^{2} = \frac{\mu}{2} \sum_{j} \dot{q}_{j}^{2} \varepsilon$$

$$(5.1)$$

Again let me jump quickly ahead and remind you of the definition of the Stieltjes integral:

$$\int f(x)dx = \lim_{\Delta x \to 0} \sum_{j} f(x_j) \Delta x.$$
(5.2)

So you see that if we take the limit $\varepsilon \to 0$ in (5.1), it is like the limit $\Delta x \to 0$ in (5.2), and the sum in (5.1) will turn into an integral. So it's good that we have an ε at the right place.

Back to the story. As you know, the potential energy of a spring is proportional to the square of the stretching of the spring. The springs are unstretched when $q_{j+1} - q_j = 0$, the system is at rest then. As the heights of the masses j and j + 1 starts to differ a little, the stretching of the spring between mass j and mass j + 1 will be proportional to $(q_{j+1} - q_j)$. What about the spring constant k? Try the following experiment at home: take a spring, and cut it in half. You'll find that it is much harder to stretch the smaller spring a centimeter than it was to stretch the long spring a centimeter. Similarly if we take one of our springs, and replace them by two springs of half the length (to introduce an additional mass point), the spring constants of each of these half-length springs is double that of the long spring. The spring constant is inversely proportional to ε , and we can write $k = \kappa/\varepsilon$ with κ some material parameter. With these insights, we can write the total potential energy as

$$U = \frac{1}{2} \sum_{j} k \left(q_j - q_{j-1} \right)^2 = \frac{\kappa}{2} \sum_{j} \left(\frac{q_j - q_{j-1}}{\varepsilon} \right)^2 \varepsilon$$
(5.3)

For the last equality, we plugged in $k = \kappa/\varepsilon$ and multiplied numerator and denominator by ε . The total Lagrangian L = T - U is given by

$$L(q_1 \dots q_N, \dot{q}_1 \dots \dot{q}_N) = \frac{\mu}{2} \sum_j \dot{q}_j^2 \varepsilon - \frac{\kappa}{2} \sum_j \left(\frac{q_j - q_{j-1}}{\varepsilon}\right)^2 \varepsilon$$
(5.4)

Let's work out the Lagrangian equations of motion. In order not to make
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mistakes with the indices, let us find the equation for q_5 , so for j = 5:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_5} = \frac{\partial L}{\partial q_5} \tag{5.5}$$

The left hand side is just $\mu \varepsilon \ddot{q}_5$. For the right hand side, we have two terms contributing: the one with $(q_5 - q_4)^2$ and the one with $(q_6 - q_5)^2$. They give

$$\mu \varepsilon \ddot{q}_5 = -\frac{\kappa}{\varepsilon} \left[(q_5 - q_4) + (q_5 - q_6) \right]$$
 (5.6)

$$\Leftrightarrow \quad \ddot{q}_5 = \frac{\kappa}{\mu} \frac{q_6 - 2q_5 + q_4}{\varepsilon^2} \tag{5.7}$$

From this it is easy to get the general pattern

$$\ddot{q}_j = \frac{\kappa}{\mu} \frac{q_{j+1} - 2q_j + q_{j-1}}{\varepsilon^2}$$
(5.8)

If we label the masses q_x rather than q_j , then we have $q_{x-\varepsilon}$ for q_{j-1} since the x coordinate of point j-1 lies an amount ε to the left of point j. Now we're finally going to treat x as a continuum index – and to emphasize this we are going to change the latin q_x to a greek letter $\varphi(x)$. So,

$$\lim_{\varepsilon \to 0} \frac{q_j - q_{j-1}}{\varepsilon} \to \lim_{\varepsilon \to 0} \frac{\varphi(x) - \varphi(x - \varepsilon)}{\varepsilon} = \frac{\partial \varphi}{\partial x}$$
(5.9)

and

$$\lim_{\varepsilon \to 0} \frac{q_{j+1} - 2q_j + q_{j-1}}{\varepsilon}$$

$$\to \quad \lim_{\varepsilon \to 0} \frac{\varphi(x+\varepsilon) - 2\varphi(x) + \varphi(x-\varepsilon)}{\varepsilon^2} = \frac{\partial^2 \varphi}{\partial x^2} \tag{5.10}$$

In this limit, expression (5.8) becomes a field equation

$$\frac{\partial^2 \varphi}{\partial t^2} = \frac{\kappa}{\mu} \frac{\partial^2 \varphi}{\partial x^2} \tag{5.11}$$

This is the wave equation, with wave velocity $c = \sqrt{\kappa/\mu}$. The vertical displacement on the string will be wave-like. Note that if we hadn't put the ε 's in the right place in the masses and spring constants in the original problem, we would have still ε 's in the wave velocity – the theory would not have generated a good field theory. This is an important point to keep in mind: the constants of the theory depend on the scale of the mesh, an idea which you also have encountered when studying renormalization in the advanced statistics master course.

5.2 Field Lagrangian

What happens to the Lagrangian (5.4) if we take the continuum limit? As mentioned above, the sums become integrals. The kinetic energy becomes

$$\lim_{\varepsilon \to 0} \frac{\mu}{2} \sum_{j} \dot{q}_{j}^{2} \varepsilon = \int \frac{\mu}{2} \left(\frac{\partial \varphi}{\partial t}\right)^{2} dx, \qquad (5.12)$$

and the potential energy becomes

$$\lim_{\varepsilon \to 0} \frac{\kappa}{2} \sum_{j} \left(\frac{q_j - q_{j-1}}{\varepsilon} \right)^2 \varepsilon = \int \frac{\kappa}{2} \left(\frac{\partial \varphi}{\partial x} \right)^2 dx.$$
(5.13)

This brings us to the field Lagrangian

$$L\left(\varphi, \frac{\partial\varphi}{\partial t}, \frac{\partial\varphi}{\partial x}\right) = \frac{\kappa}{2} \int \left[\frac{1}{c^2} \left(\frac{\partial\varphi}{\partial t}\right)^2 - \left(\frac{\partial\varphi}{\partial x}\right)^2\right] dx \tag{5.14}$$

You see that this field Lagrangian depends on the derivatives of the field with respect to time and position. In principle it could also depend on the field itself, for example if you have a gravitational potential $\propto q_j$ you'll get a term $\propto \varphi$ in the field Lagrangian.

The action functional

$$S = \int L(q_1 \dots q_N, \dot{q}_1 \dots \dot{q}_N) dt$$
(5.15)

will in the continuum limit become

$$S = \frac{\kappa}{2} \int \left[\frac{1}{c^2} \left(\frac{\partial \varphi}{\partial t} \right)^2 - \left(\frac{\partial \varphi}{\partial x} \right)^2 \right] dx dt$$
 (5.16)

This is a nice spacetime integral. The term in between square brackets is (up to an irrelevant scaling constant) called the *Lagrangian density*,

$$\mathcal{L}\left(\varphi, \frac{\partial\varphi}{\partial t}, \frac{\partial\varphi}{\partial x}\right) = \frac{1}{2} \left(\frac{\partial\varphi}{\partial\left(ct\right)}\right)^{2} - \frac{1}{2} \left(\frac{\partial\varphi}{\partial x}\right)^{2}$$
(5.17)

5.2.1 Relativistic notations

Now it's time to go from 1D plus time to 4D spacetime. In special relativity, we want to treat space and time on equal footing, and this will be reflected in the notations that we will use. As pointed out in the previous chapter, I will use notations with Greek indices μ to denote the coefficients of the position $x^{\mu} = \{x^0, x^1, x^2, x^3\} = \{ct, x, y, z\}$ and the derivatives with respect to them

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 $\partial_{\mu}f = \partial f/\partial x^{\mu}$. My metric convention is $\{1, -1, -1, -1\}$, so I set c = 1 from hereon after.

The Lagrangian density depends on φ and the four derivatives $\partial_{\mu}\varphi$,

$$\mathcal{L}(\varphi, \partial_{\mu}\varphi). \tag{5.18}$$

Our special example of a 1D string could also be extended to a 3D mattress and written as $\mathcal{L}(\varphi, \partial_{\mu}\varphi) = (1/2)\partial^{\mu}\varphi \ \partial_{\mu}\varphi$ in this notation. Forget x as a coordinate: we will use use $x = \{\vec{x}, t\}$ to denote a spacetime point. The Lagrangian density takes the value of the field and its derivatives at a given spacetime point and returns a number. Integrated over all spacetime, this gives you a single number that you can associate with a particular realization $\varphi(\vec{x}, t) = \varphi_x$ of the entire field,

$$S[\varphi] = \int dx \, \mathcal{L}(\varphi, \partial_{\mu}\varphi).$$
(5.19)

Remember that $\int dx$ now has to integrate over all of spacetime, not just one coordinate.

REMARK – The discrete grid viewpoint for fields is a useful mental tool, and it will be helpful if you can move back and forth between the discrete and continuous versions easily. In fact, "finite element methods" or "lattice QCD" does exactly this: it solves the field equations by discretizing them on a mesh. We can also discretize our relativistic field Lagrangian. To do that we need to replace our 1D grid plus time to a 2D spacetime grid. Sometimes, for simplicity, I imagine a very simple finite spacetime with just five positions in space and five times called the "simpleverse" in contrast with the difficult universe. A scalar field φ_x on the simpleverse is a collection of 25 numbers, indexed by $x = \{ct, \mathbf{x}\}$. We could use an index i = 1, 2, 3, ..., 25 but since we know that spacetimes have a special structure we keep $x = \{i, j\}$ with now i = 1..5 and j = 1..5. The analogy between generalized coordinates $q_{i,j}$ and φ_x is obvous. For each realization of the field, each set of 25 input numbers, you can calculate a score $S[\varphi_x]$. Expression (5.19) tells us that the action can be written as a sum over all the spacetime points $x = \{i, j\}$ of some Lagrangian function which depends only on the value of the field in that spacetime point $\varphi_x = q_{i,j}$, and the difference $\partial_\mu \varphi$ with the values in neighbouring points (i.e. $\partial_i \varphi = (q_{i+1,j} - q_{i,j}) / \varepsilon$). Such action functionals are called "local".

5.3 Classical field equations

The link between this action functional and the classical equations of motion for the fields are found by extremizing the action. If $\tilde{\varphi}_x$ is the field configuration that extremizes the action S, then the value of the action should not change if we add a small change $\delta \varphi$ to the field $\tilde{\varphi}$. In other words,

$$\delta S = S[\tilde{\varphi} + \delta \varphi] - S[\tilde{\varphi}] \tag{5.20}$$

is zero up to first order in $\delta\varphi_x$ if $\tilde\varphi_x$ is the field configuration that extremizes S. Since

$$\partial_{\mu}\left(\tilde{\varphi} + \delta\varphi\right) = \partial_{\mu}\tilde{\varphi} + \partial_{\mu}\left(\delta\varphi\right) \tag{5.21}$$

we see that adding a change $\delta \varphi$ to $\tilde{\varphi}$ implies that we add $\partial_{\mu} (\delta \varphi)$ to $\partial_{\mu} \tilde{\varphi}$. We can now relate the change in the action functional to the change in the Lagrangian density, by using the chain rule:

$$\delta S = \delta \left\{ \int dx \, \mathcal{L}(\varphi, \partial_{\mu}\varphi) \right\}$$
$$= \int \left(\frac{\partial \mathcal{L}}{\partial \tilde{\varphi}} \delta \varphi + \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \tilde{\varphi})} \partial_{\mu} \left(\delta \varphi \right) \right) dx \qquad (5.22)$$

Now we use partial integration to simplify the second term:

$$\int \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \tilde{\varphi})} \partial_{\mu} (\delta \varphi) \, dx = \left. \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \tilde{\varphi})} \delta \varphi \right|_{edge} - \int \delta \varphi \, \partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \tilde{\varphi})} \right) dx \qquad (5.23)$$

The boundary term drops out usually (but not necessarily always) as we fix the boundary conditions there, so $\delta \varphi_{x \in edge} = 0$ at the edge. The change in the action then becomes

$$\delta S = \int \left[\frac{\partial \mathcal{L}}{\partial \tilde{\varphi}} - \partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \tilde{\varphi})} \right) \right] \delta \varphi dx \tag{5.24}$$

The only way that this can be zero for all $\delta \varphi$ is if the field $\tilde{\varphi}$ satisfies the following field equation:

$$\partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu} \tilde{\varphi} \right)} \right) = \frac{\partial \mathcal{L}}{\partial \tilde{\varphi}}$$
(5.25)

Just to make sure you remember Einstein summation and our metric convention, I'll write out the left hand side for you in our old notation:

$$\partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \tilde{\varphi})} \right) = \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{t} \tilde{\varphi})} \right) - \frac{\partial}{\partial x} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{x} \tilde{\varphi})} \right) \\ - \frac{\partial}{\partial y} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{y} \tilde{\varphi})} \right) - \frac{\partial}{\partial z} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{z} \tilde{\varphi})} \right)$$
(5.26)

Remark – At this point, we can also introduce the field canonically conjugated to φ . We call this π in honor of the canonical momentum p and Greek culture. The definition of this field is

$$\pi = \frac{\partial \mathcal{L}}{\partial \left(\partial_0 \varphi\right)} \tag{5.27}$$

where the right hand side is evaluated in x. With this canonically conjugated field we can introduce the field Hamiltonian density:

$$\mathcal{H}(\varphi,\pi) = \pi \partial_0 \varphi - \mathcal{L}(\varphi,\partial_\mu \varphi) \tag{5.28}$$

It is called a density because this is again a local quantity: it only depends on the values of the fields φ (and its spatial derivatives) and π in the point x in which you want to calculate the Hamiltonian density.

5.4 Example: Klein-Gordon scalar field

As a simple example, let's look at a scalar field φ that associates a real or a complex number to each point in spacetime. What is the most general Lagrangian that we can make that

- 1. has up to second powers of the derivatives in the fields, and
- 2. is Lorentz invariant?

The question you just read is typical of how theoretical physicists make models. The first requirement asks for simplicity – often equated to elegance of the theory, but if we're honest about it, we have to admit that we can only solve linear equations of motion, so we don't want higher powers in the field Lagrangian. The second requirement is a certain symmetry. "Modelling" in theoretical physics is different from modelling in fashion, and in physics often comes down to choosing which symmetries should be obeyed. Lorentz invariance doesn't seem to very outlandish to ask for if we want to make a model that agrees with special relativity!

Scalars and four-vectors are Lorentz-invariant. Here we have $\partial_{\mu}\varphi$ as a (covariant) four-vector, and φ itself as a scalar. The Lagrangian density itself is a scalar. So we're pretty limited in our options, we can use φ, φ^2 or we have to construct a scalar from $\partial_{\mu}\varphi$. The only way of doing this is

$$\partial^{\mu}\varphi\partial_{\mu}\varphi = \partial_{\mu}\varphi \ g^{\mu\nu} \ \partial_{\nu}\varphi \tag{5.29}$$

$$= (\partial_t \varphi)^2 - (\partial_x \varphi)^2 - (\partial_y \varphi)^2 - (\partial_z \varphi)^2. \qquad (5.30)$$

With these, it is clear that the most general Lagrangian density agreeing with the two above requirements is

$$\mathcal{L} = \frac{1}{2} \partial^{\mu} \varphi \ \partial_{\mu} \varphi - \frac{m^2}{2} \varphi^2 \tag{5.31}$$

Here, m^2 is the only parameter, reflecting the ration of the coefficient in front of φ^2 to the coefficient in front of $\partial^{\mu}\varphi \ \partial_{\mu}\varphi$. We could still include a term linear in φ (and a second parameter), and write $\frac{m}{2}(\varphi - a)^2$ for the last term, but I'll leave out that bit of extra generality for the sake of clarity. Next, we determine the field equations corresponding to this Lagrangian. For this, we calculate first the right hand side of equation (5.25), starting with

$$\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi)} = \frac{\partial}{\partial (\partial_{\mu} \varphi)} \left(\frac{1}{2} g^{\lambda \nu} \partial_{\lambda} \varphi \partial_{\nu} \varphi \right)$$
$$= \frac{1}{2} g^{\mu \nu} \partial_{\nu} \varphi + \frac{1}{2} g^{\lambda \mu} \partial_{\lambda} \varphi$$
$$= \partial^{\mu} \varphi.$$

Note moreover that the time-component of this is the canonically conjugated field

$$\pi = \frac{\partial \mathcal{L}}{\partial (\partial_0 \varphi)} = \partial^0 \varphi$$

$$\Rightarrow \mathcal{H}(\varphi, \pi) = \pi \partial_0 \varphi - \mathcal{L}$$

$$\Rightarrow \mathcal{H}(\varphi, \pi) = \frac{1}{2} \left[\pi^2 + (\partial_x \varphi)^2 + (\partial_y \varphi)^2 + (\partial_z \varphi)^2 \right] + \frac{m}{2} \varphi^2.$$

We leave the Hamiltonian out of it, so this was just a side remark. Continuing with the calculation of the equation of motion, we find that

$$\partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu} \varphi \right)} \right) = \partial_{\mu} \partial^{\mu} \varphi \tag{5.32}$$

This Lorentz invariant second derivatives is the d'Alembertian, denoted by a square,

$$\Box \varphi = \partial_{\mu} \partial^{\mu} \varphi = \partial_{t}^{2} \varphi - \partial_{x}^{2} \varphi - \partial_{y}^{2} \varphi - \partial_{y}^{2} \varphi$$
(5.33)

It is named after Jean le Rond d'Alembert, a French philosopher and mathematician living in the eighteeth century and who is most famous among laypeople for the encyclopedia he compiled together with Denis Diderot. He was the illegitimate child of an aristocrat and choose a name with a little 'd' to reflect this. First he wanted to be d'Aremberg, like the science campus of the KULeuven. He invented the derivative, defining it as a limit. Someone must have thought a square is a logical choice for the operation of d'Alembert since the spatial (3D) Laplacian is a triangle. Anyway, we've found that the right hand side of equation (5.25) is the d'Alembertian. The right hand side is simpler and elicits less historical comments:

$$\frac{\partial \mathcal{L}}{\partial \varphi} = -m^2 \varphi \tag{5.34}$$

Hence, the field equation becomes

$$\Box \varphi + m^2 \varphi = 0 \tag{5.35}$$

This is known as the Klein-Gordon equation¹ (for $m \neq 0$), and it is simply the wave equation (5.11) when m = 0. The "speed of the wave" is of course the

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 $^{^{1}}$ It could equally have been called the "de Donder" equation, after the Belgian physicist Théophile Ernest De Donder who formulated it at the same time as Klein and Gordon, but who has less luck at promoting his name.

light velocity c that we chose equal to one to specify our units of time (see again appendix A).

In this course, I expect you to be able to solve such partial differential equations for straightforward boundary conditions, mastering methods such as separation of variables, Green's functions, and other tools you have seen in the course of classical field theory. If you don't remember that, read your old course again!

5.5 Transformations

5.5.1 Coordinate transformations

Next we look at the effect of coordinate transformations on the fields. To do this, we focus on translations

$$x^{\mu} \to \tilde{x}^{\mu} = x^{\mu} + a^{\mu} \tag{5.36}$$

The tilde indicates the new coordinates. You've taken your old reference frame and moved its origin over to the spacetime point -a, keeping the axis parallel. For the fields we have

$$\varphi(x^{\mu}) \to \varphi(\tilde{x}^{\mu}) = \varphi(x^{\mu} + a^{\mu}) \tag{5.37}$$

The field stays draped the same way over spacetime, only the coordinates that you choose to label the spacetime points has changed. Two successive translations can be combined into one translation. This operation of combining translations brings the structure of a Lie group to the set of possible translations – I remind you that a Lie group or "continuous" group is a group whose elements are indexed by a set of continuous parameters (such as angles or displacements), such that the identity element corresponds to the zero value of the parameters. As is suitable for Lie groups, we look at the effect of a very small step $x^{\mu} \to x^{\mu} + \varepsilon^{\mu}$ with ε infinitesimal. Then we can use a Taylor series expansion

$$\varphi(x^{\mu}) \to \varphi(\tilde{x}^{\mu}) = \varphi(x^{\mu} + \varepsilon^{\mu}) = \varphi(x^{\mu}) + \varepsilon^{\mu} \partial_{\mu} \varphi + \mathcal{O}((\varepsilon)^{2})$$
(5.38)

So, the effect on the field is to add a small perturbation $\delta \varphi$ like the ones we considered to derive the field equations. For infinitesimal translations, the change in the field is given by

$$\delta\varphi = \varepsilon^{\mu}\partial_{\mu}\varphi \tag{5.39}$$

Question: can we rewrite this as

$$\varphi(x^{\mu}) \to \varphi(\tilde{x}^{\mu}) = \left(\hat{1} + i\varepsilon \hat{X}\right)\varphi(x^{\mu})$$
 (5.40)

where $\hat{1}$ is the identity operator and \hat{X} is an operator that transforms the field (so $\delta \varphi = i \varepsilon \hat{X}[\varphi]$)? This operator is called the generator of the group, as we discussed in the review on group theory, and ε is the group parameter for an infinitesimal step. Here we should consider \hat{X} to be a covariant vector,

$$i\varepsilon^{\mu} \hat{X}_{\mu}[\varphi] = \varepsilon^{\mu} \partial_{\mu} \varphi$$

$$\Leftrightarrow \quad \hat{X}_{\mu} = -i\partial_{\mu}$$
(5.41)

This will later be linked to the quantum mechanical momentum operator, which is the generator for translations. If the field equations of the system remain the same after performing a translation, we say that the system has a symmetry: it is translationally invariant.

Let's look at some other coordinate transformations – I leave it as exercises to find the generators:

• Scale changes: $x^{\mu} \to \tilde{x}^{\mu} = \alpha x^{\mu}$. The infinitesimal rescaling is $(1 + \varepsilon)x^{\mu}$, and the effect on the field is

$$\varphi(\tilde{x}^{\mu}) = \varphi\left[(1+\varepsilon)x^{\mu}\right] = \varphi(x^{\mu}) + \varepsilon x^{\mu}\partial_{\mu}\varphi \qquad (5.42)$$

so that the generator for scale changes is the scalar

$$\hat{X}^{scaling} = -ix^{\mu}\partial_{\mu} \tag{5.43}$$

• Rotations: $x^{\mu} \to \tilde{x}^{\mu} = M^{\mu}_{\nu} x^{\mu}$ with M the rotation matrix. The generator is a rank 2 covariant tensor, the angular momentum

$$L_{\mu\nu} = -i \left(x_{\mu} \partial_{\nu} - x_{\nu} \partial_{\mu} \right) \tag{5.44}$$

• Special conformal map: this is a kind of map that conserves angles between curves,

$$\tilde{x}^{\mu} = \frac{x^{\mu} - b^{\mu} x^2}{1 - 2(b_v x^v) + b x^2}.$$
(5.45)

its generator is

$$\hat{K}_{\mu} = -i\left(2x_{\mu}x^{\nu}\partial_{\nu} - x^{2}\partial_{\mu}\right) \tag{5.46}$$

• Conformal maps: these are coordinate transformations that leave the metric invariant up to a local scaling factor. You can imagine that a theory satisfying general relativity should be invariant with respect to such transformations. A map $x^{\mu} \to \tilde{x}^{\mu} = f(x^{\mu})$ will transform the metric according to

$$g_{\mu\nu}(x) \to \tilde{g}_{\mu\nu}(x) = \frac{\partial x^{\alpha}}{\partial \tilde{x}^{\mu}} \frac{\partial x^{\beta}}{\partial \tilde{x}^{\nu}} g_{\alpha\beta} \left[f^{-1}(x) \right]$$
 (5.47)

So the map f is conformal if it has an inverse and if

$$\tilde{g}_{\mu\nu}(x) = \Omega^2(x)g_{\mu\nu}(x) \tag{5.48}$$

Examples of this very broad class of maps include translations, rotations, scalings, Lorentz-boosts,... This large set of maps forms the conformal group. Field theories invariant to these transformations are called "conformal field theories" (CFT). They have gained importance recently due to the Maldacena theorem that says that a theory with gravitation in some bulk volume (and Anti-de Sitter space, AdS) is equivalent to a conformal field theory living on the surface of that volume, without gravity (this is also known as the AdS-CFT correspondence).

5.5.2 Component transformations

Up till now we only considered scalar fields, where to every spacetime point a scalar is assigned. However, more complicated objects may be attached to spacetime points. For example, we could assign spinors representing spin-up or spin-down for for spin-1/2 particles, such as

$$\eta_{+} = \begin{pmatrix} 1\\0 \end{pmatrix} \qquad \eta_{-} = \begin{pmatrix} 0\\1 \end{pmatrix}, \qquad (5.49)$$

to spacetime points². The theory could then be invariant under transformations that swap or mix the *components* of the spinors – we'll call this an *internal* symmetry. For example, the theory could be invariant to applying to each spinor $\eta(x)$ a unitary transformation $\hat{U}[\eta(x)]$. This means we multiply the rank-2 column vector with a 2 × 2 unitary matrix to get the transformed rank-2 column vector. Unitarity means that $\hat{U}^{\dagger}\hat{U} = \hat{1}$. If you apply two unitary transformations in succession, the result can be expressed as a single unitary transformation. The unitary transformations form a Lie group, denoted as U(n) if we have $n \times n$ dimensional matrices. If we moreover demand that these matrices have determinant equal to one, we get at subgroup, called the "special unitary group", or SU(n).

The elements of SU(2) will mix up the components of rank-2 spinors. Such elements can be written as

$$\begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \text{ with } a, b \in \mathbb{C} \text{ and } |a|^2 + |b|^2 = 1.$$
 (5.50)

The generators of SU(2) are the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(5.51)

In general, SU(n) has $n^2 - 1$ generators. We'll get back to this interesting group and its generators in later chapters, here I wanted to emphasize that for fields

²Don't be fooled: it is not because we attach a multicomponent object to every spacetime point that we have a quantum field theory! Complex tensors or multicomponent fields can be classical fields as well – we'll see later what makes it "quantum".

that assign more complicated objects to spacetime points, you have more than just the coordinate transformations. We'll get back to component transformations (and give a simple example) when we look at gauge transformations.

5.6 Symmetry of a field theory

A symmetry of a field theory is a transformation that leaves the field equations invariant.

We go back to our example of a transformation: the translation

$$x^{\mu} \rightarrow \tilde{x}^{\mu} = x^{\mu} + a^{\mu} \tag{5.52}$$

$$\varphi(x^{\mu}) \rightarrow \varphi(x^{\mu}) + \underbrace{a^{\mu}\partial_{\mu}\varphi}_{\delta_{\mu}\varphi} + \mathcal{O}(a^2)$$
 (5.53)

Now that we have figured out the consequence for the coordinates and for the fields, we want to figure out the effect of the transformation on the Lagrangian density next.

On the one hand, we have

$$\delta \mathcal{L} = \frac{\partial \mathcal{L}}{\partial \varphi} \delta \varphi + \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi)} \partial_{\mu} \left(\delta \varphi \right)$$
(5.54)

That is quite similar to what we used when deriving the field equations. If the field φ satisfies the field equation, we can moreover replace

$$\frac{\partial \mathcal{L}}{\partial \varphi} = \partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu} \varphi \right)} \right) \tag{5.55}$$

in the first term on the right-hand-side of (5.54) and get

$$\delta \mathcal{L} = \partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi)} \right) \ \delta \varphi + \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi)} \ \partial_{\mu} \left(\delta \varphi \right) \tag{5.56}$$

We recognise the product rule for derivatives, so we can write

$$\delta \mathcal{L} = \partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi)} \delta \varphi \right) \tag{5.57}$$

So, if the Lagrangian density is invariant under the transformation, the expression between brackets is conserved. For translations we have $\delta \varphi = a^{\mu} \partial_{\mu} \varphi$, so

$$\delta \mathcal{L}_{transl} = a^{\nu} \partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi)} \partial_{\nu} \varphi \right)$$
(5.58)

On the other hand, we could consider the explicit coordinate dependence of the Lagrangian density of the classical field – for every point in spacetime, the Lagrangian density can be evaluated and gives back a scalar. So we have, just like for scalar fields,

$$\delta \mathcal{L}_{transl} = a^{\mu} \partial_{\mu} \mathcal{L} \tag{5.59}$$

Equating the two results (5.58) and (5.59) gives

$$a^{\mu}\partial_{\mu}\mathcal{L} = a^{\nu}\partial_{\mu}\left(\frac{\partial\mathcal{L}}{\partial(\partial_{\mu}\varphi)}\partial_{\nu}\varphi\right)$$
(5.60)

Now we can use that

$$a^{\mu}\partial_{\mu}\mathcal{L} = \left(\delta^{\mu}_{,\nu}a^{\nu}\right)\partial_{\mu}\mathcal{L} = a^{\nu}\partial_{\mu}\left(\delta^{\mu}_{,\nu}\mathcal{L}\right)$$
(5.61)

to rewrite (5.60) as

$$a^{\nu}\partial_{\mu}\left(\frac{\partial\mathcal{L}}{\partial\left(\partial_{\mu}\varphi\right)}\partial_{\nu}\varphi - \delta^{\mu}_{.\nu}\mathcal{L}\right) = 0$$
(5.62)

This must hold for all a, so we have a conservation law. The expression between brackets,

$$T^{\mu}_{.\nu} = \frac{\partial \mathcal{L}}{\partial (\partial_{\mu}\varphi)} \partial_{\nu}\varphi - \delta^{\mu}_{.\nu}\mathcal{L}$$
(5.63)

is conserved. It is called the *energy-momentum tensor*. We get

$$\partial_{\mu}T^{\mu.}_{.\nu} = 0 \tag{5.64}$$

Example – Let's calculate this for the Klein-Gordon Lagrangian that we used before, $\mathcal{L}(\varphi, \partial_{\mu}\varphi) = (1/2)\partial_{\mu}\varphi\partial^{\mu}\varphi - (m^2/2)\varphi^2$. For this Lagrangian, we had

$$\frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu}\varphi\right)} = \partial^{\mu}\varphi \tag{5.65}$$

so that

$$T^{\mu.}_{.\nu} = \partial^{\mu}\varphi\partial_{\nu}\varphi - \delta^{\mu.}_{.\nu} \left[\frac{1}{2}\partial_{\mu}\varphi\partial^{\mu}\varphi - \frac{m^{2}}{2}\varphi^{2}\right]$$
$$= \partial^{\mu}\varphi\partial_{\nu}\varphi \left(1 - \frac{1}{2}\delta^{\mu.}_{.\nu}\right) + \frac{m^{2}}{2}\varphi^{2}\delta^{\mu.}_{.\nu}$$
(5.66)

Let's look at some specific components:

$$T_{.0}^{0.} = \frac{\partial \mathcal{L}}{\partial (\partial_0 \varphi)} \partial_0 \varphi - \mathcal{L}$$

= $\pi \ \partial_0 \varphi - \mathcal{L} = \mathcal{H}$ (5.67)

We used equations (5.27) and (5.28). The time-time component is the Hamiltonian density or energy density which is sometimes noted as ρ_E . The time-component of our conservation law,

$$\partial_{\mu}T_{.0}^{\mu.} = 0 \tag{5.68}$$

can be interpreted as a continuity equation

$$\frac{d\rho_E}{dt} + \boldsymbol{\nabla} \cdot \mathbf{j}_E = 0 \tag{5.69}$$

for the energy density. This also implies that $T_{.0}^{i}$ with i = 1, 2, 3 is the momentum density – the total momentum being $P^{i} = \int dx T_{.0}^{i}$. This is the reason why $T_{.\nu}^{\mu}$ is called the energy-momentum tensor.

Coordinate transformations and the component transformations that we have seen form continuous groups, and may lead to *continuous symmetries*. We also have *discrete symmetries*, such as parity. The field equations could be invariant with respect to

$$\varphi(x) \to \hat{P}[\varphi(x)] = \varphi(-x).$$
 (5.70)

If we apply \hat{P} again, we get the identity. So this is a very simple group – with a countable number of elements, here even a finite number of elements.

5.7 Conserved currents and charges

How about the effect of transformations on the action functional

$$S_V = \int_V \mathcal{L}\left(\varphi, \partial_\mu \varphi\right) dx, \qquad (5.71)$$

Note that we pick a 4-volume of spacetime for our present purposes, and this does not have to be an infinitely large region. In fact, we'll be interested at what happens at the boundary of any given volume. That's why I put a subscript V in the action functional defined here.

From the previous section, we know the effect of a transformation on the Lagrangian density, so we just plug in that result (expression (5.54)):

$$\delta S_V = \int_V \delta \mathcal{L} dx = \int_V \left[\frac{\partial \mathcal{L}}{\partial \varphi} \delta \varphi + \frac{\partial \mathcal{L}}{\partial (\partial_\mu \varphi)} \partial_\mu (\delta \varphi) \right] dx$$
(5.72)

Partial integration, performed on the second term between square brackets, yields

$$\delta S_V = \int\limits_V \left[\frac{\partial \mathcal{L}}{\partial \varphi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial (\partial_\mu \varphi)} \right] \delta \varphi dx + \left. \frac{\partial \mathcal{L}}{\partial (\partial_\mu \varphi)} \delta \varphi \right|_{boundary}$$
(5.73)

The term between square brackets is just the equation of motion, so that becomes zero and we have

$$\delta S_V = \left. \frac{\partial \mathcal{L}}{\partial \left(\partial_\mu \varphi \right)} \delta \varphi \right|_{boundary} \tag{5.74}$$

5.7. CONSERVED CURRENTS AND CHARGES

If the action functional is invariant with respect to the transformation, $\delta S_V = 0$ for any choice of the 4-volume V. If we take a tiny cube, then we this says that what comes in from any side must leave the cube as well. This leads to

$$\forall V : \delta S_V = 0 \Rightarrow \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\mu \varphi)} \delta \varphi \right) = 0$$
 (5.75)

The quantity between brackets can be identified with a current

$$J^{\mu} = \frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu}\varphi\right)} \delta\varphi \tag{5.76}$$

which is conserved,

$$\partial_{\mu}J^{\mu} = 0 \tag{5.77}$$

Note that we can write in "old notation" $J = \{J^0, J^1, J^2, J^3\} = \{\rho, j_x, j_y, j_z\}$ and identify ρ with a "charge density" and j_x, j_y, j_z with the associated current density in 3-space. In this notation, $\partial_{\mu}J^{\mu} = 0$ is equivalent to the continuity equation $\partial \rho / \partial t + \nabla \cdot \mathbf{j} = 0$. This implied charge conservation, not in the sense that the charge density can never change, but in the following sense: when you see the charge decrease somewhere and increase in another place, the only whay that could have happened is if change density has been flowing from one to the other place. That is the meaning of the continuity equation, and that is what we mean when we say there is a "conserved 4-current". We already encountered an example in the previous section: the energy-momentum tensor represents 4 conserved currents. For the "zero" component the conserved charge is the energy density, for the other components it is momentum density.

In this section we have a fully general result, valid for any continuous transformation. This result was first derived by Emmy Noether, and is known as

Noether's theorem: For each continuous
symmetry that leaves the theory invariant,
there exists a conserved current:
$$J^{\mu} = \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi)} \delta \varphi$$
(5.78)

We saw that modeling in theoretical physics often comes down to selecting the right symmetries of the system. Noether's theorem gives a very important clue for setting up theories: the correct symmetries are linked to conserved quantities!

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Chapter 6

Gauge theories

These kind of theories play a very important role in particle physics. As it turns out, nature¹ seems to have picked local gauge invariance as one of the symmetries to fix the model.

6.1 Gauge transformations

In our earlier example, we consider a Klein-Gordon Lagrangian for a single, real field. Let's look at the case with two fields, φ_R and φ_I , and just assume they both obey the Klein-Gordon Lagrangian density:

$$\mathcal{L}(\varphi_R,\varphi_I,\partial_\mu\varphi_R,\partial_\mu\varphi_I) = \frac{1}{2}\partial_\mu\varphi_R\partial^\mu\varphi_R - \frac{m^2}{2}\varphi_R^2 + \frac{1}{2}\partial_\mu\varphi_I\partial^\mu\varphi_I - \frac{m^2}{2}\varphi_I^2$$
(6.1)

What kind of symmetries do we have? Lorentz invariance is one of them. We could also swap

$$\varphi_R, \varphi_I \longleftrightarrow \varphi_I, \varphi_R \tag{6.2}$$

and that would not change the Lagrangian. However, there are more ways to mix the components, leaving the Lagrangian invariant! To see this, use both real fields to construct a complex field:

$$\phi = \frac{\varphi_R + i\varphi_I}{\sqrt{2}}.\tag{6.3}$$

From this point of view, we assign to each spacetime point a single complex number rather than two real numbers. It's clear that we can use this to simplify the mass term, since

$$\varphi_R^2 + \varphi_I^2 = 2\phi^*\phi \tag{6.4}$$

¹You may substitute the name of your favorite god here. Antwerp University is pluralist.

How about the kinetic term, can we write $\partial_{\mu}\phi^*\partial^{\mu}\phi$? Let's see

$$2\partial_{\mu}\phi^{*}\partial^{\mu}\phi = \partial_{\mu}\left(\varphi_{R} - i\varphi_{I}\right)\partial^{\mu}\left(\varphi_{R} + i\varphi_{I}\right)$$
$$= \partial_{\mu}\varphi_{R}\partial^{\mu}\varphi_{R} + \partial_{\mu}\varphi_{I}\partial^{\mu}\varphi_{I}$$
$$+ i\left(\partial_{\mu}\varphi_{R}\partial^{\mu}\varphi_{I} - \partial^{\mu}\varphi_{R}\partial_{\mu}\varphi_{I}\right)$$
(6.5)

The last terms cancel, as you can show by pumping around some indices. So we get

$$\mathcal{L}(\phi,\partial_{\mu}\phi) = \partial^{\mu}\phi^{*}\partial_{\mu}\phi - m^{2}\phi^{*}\phi \tag{6.6}$$

This reveals yet another *continuous* symmetry of the system:

$$\phi \to \phi e^{i\theta} \tag{6.7}$$

leaves the Lagrangian unchanged for any value of the parameter θ (giving you a continuum of possible choices). This is a U(1) unitary component transformation called a *gauge transformation*. You can measure the phase from any chosen global angle, that choice is the gauge. Note that the phase θ should be a constant, if it depends on position, we get into trouble. It's very instructive to investigate this trouble in more detail.

REMARK – In quantum mechanics, transformations are related to unitary operators. These are heralds of symmetry, as they often leave expectation values unchanged. Let's consider a complex field ϕ . For these fields, the unitary transformation acts as follows

$$\phi \rightarrow \hat{U}\phi$$
 (6.8)

$$\phi^{\dagger} \rightarrow \phi^{\dagger} \hat{U}^{\dagger} \tag{6.9}$$

Now ϕ could just be a complex-valued scalar, in which case the daggers become complex conjugates, and unitary transformations are represented by a complex number with modulus 1. This means that the elements of U(1) can be written as $e^{i\theta}$ with θ real. Indeed, $\hat{U}^{\dagger}\hat{U} = e^{-i\theta}e^{i\theta} = 1$. That is what we have in our example. But if ϕ is a column vector of rank n, then ϕ^{\dagger} is a row vector of rank n containing the complex conjugates of the column components. Then we need the elements of SU(n), these are $n \times n$ unitary matrices with determinant 1.

6.2 Global gauge invariance

"Global" means that U does not depend on the position. In our example, a global U(1) transformation multiplies the complex field at every spacetime point with the same phase factor $e^{i\theta}$, as on the left hand side of the figure below. We can write this in a way that is a bit more formal and generally valid. Let's apply (6.8),(6.9) to our Lagrangian density (6.6), leaving open the possibility of a multicomponent complex field:

$$\mathcal{L} = \partial^{\mu} \phi^{\dagger} \partial_{\mu} \phi - m^2 \phi^{\dagger} \phi \tag{6.10}$$

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6.3. LOCAL GAUGE INVARIANCE

The "mass" term transforms as

$$\phi^{\dagger}\phi \rightarrow \left(\phi^{\dagger}\hat{U}^{\dagger}\right)\left(\hat{U}\phi\right) = \phi^{\dagger}\left(\hat{U}^{\dagger}\hat{U}\right)\phi = \phi^{\dagger}\phi$$
 (6.11)

The derivative transforms as

$$\partial_{\mu}\phi \to \partial_{\mu}\left(\hat{U}\phi\right) = \hat{U}\left(\partial_{\mu}\phi\right)$$
(6.12)

We can take out \hat{U} as long as we perform the same transformation in every point in spacetime – then \hat{U} is independent of position in spacetime. We get

$$\partial^{\mu}\phi^{\dagger}\partial_{\mu}\phi \to \partial^{\mu}\left(\phi^{\dagger}\hat{U}^{\dagger}\right)\partial_{\mu}\left(\hat{U}\phi\right) = \left(\partial^{\mu}\phi^{\dagger}\right)\hat{U}^{\dagger}\hat{U}\left(\partial_{\mu}\phi\right) = \partial^{\mu}\phi^{\dagger}\partial_{\mu}\phi, \quad (6.13)$$

so indeed $\mathcal L$ is invariant under global gauge transformations.

global gauge transform $\mathrm{U=}e^{\mathrm{i} heta}$	local gauge transform $\mathrm{U=}e^{\mathrm{i}\theta(\mathrm{x})}$
111111	11
111111	117->>>
777777	$\uparrow \uparrow \uparrow \neg \neg \rightarrow$
777777	11177
777777	$\nabla \uparrow \uparrow \uparrow \land \land$
7 7 7 7 7 7 <i>7</i>	1 1 1 7 7 7 7 N

arrows point in the direction of $\boldsymbol{\theta}$

6.3 Local gauge invariance

Now we look at the case where \hat{U} does depend on the position – for a scalar (complex) field such a local gauge transform is illustrated on the right hand side of the previous figure. The difference with the previous case is that (6.12) no longer holds:

$$\partial_{\mu} \left(\hat{U} \phi \right) \neq \hat{U} \left(\partial_{\mu} \phi \right) \tag{6.14}$$

In fact, we have

$$\partial_{\mu}\phi \to \partial_{\mu}\left(\hat{U}\phi\right) = \left(\partial_{\mu}\hat{U}\right)\phi + \hat{U}\left(\partial_{\mu}\phi\right)$$
$$= \hat{U}\hat{U}^{\dagger}\left(\partial_{\mu}\hat{U}\right)\phi + \hat{U}\left(\partial_{\mu}\phi\right)$$
$$= \hat{U}\left[\hat{U}^{\dagger}\left(\partial_{\mu}\hat{U}\right)\phi + \partial_{\mu}\phi\right], \qquad (6.15)$$

CHAPTER 6. GAUGE THEORIES

 \mathbf{so}

$$\partial_{\mu}\left(\hat{U}\phi\right) = \hat{U}\underbrace{\left[\partial_{\mu} + \hat{U}^{\dagger}\left(\partial_{\mu}\hat{U}\right)\right]}_{\text{this is } \neq \partial_{\mu}}\phi \qquad (6.16)$$

The operations ∂_{μ} and \hat{U} cannot be swapped as in the previous case. They do not commute, and that is the core reason why our Langrangian density (6.10) does not have local gauge invariance.

6.4 Covariant derivatives

Again, modeling is all about choosing your symmetries. So what if you want to *impose* local gauge symmetry? How should you modify your theory? In our example, we are now looking for a theory (a Lagrangian density) of a complex scalar field that (1) obeys Lorentz invariance, (2) has up to second order derivatives in the fields, and (3) has local gauge invariance.

Suppose that, in stead of the lousy ∂_{μ} , we would have another sort of derivative, lets call it D_{μ} , that commutes with \hat{U} . This would restore

$$D_{\mu}\left(\hat{U}\phi\right) = \hat{U}\left(D_{\mu}\phi\right). \tag{6.17}$$

This strange object varies along with the field so it can be taken out of \hat{U} . It is called a *co-variant derivative*. If we have such an object, we can construct a Lagrangian

$$\mathcal{L} = D^{\mu} \phi^{\dagger} D_{\mu} \phi - m^2 \phi^{\dagger} \phi \tag{6.18}$$

that obeys local gauge invariance:

$$\mathcal{L} \rightarrow D^{\mu} \left(\phi^{\dagger} \hat{U}^{\dagger} \right) D_{\mu} \left(\hat{U} \phi \right) - m^{2} \left(\phi^{\dagger} \hat{U}^{\dagger} \right) \left(\hat{U} \phi \right)$$

$$= \left(D^{\mu} \phi^{\dagger} \right) \hat{U}^{\dagger} \hat{U} \left(D_{\mu} \phi \right) - m^{2} \phi^{\dagger} \left(\hat{U}^{\dagger} \hat{U} \right) \phi$$

$$= \left(D^{\mu} \phi^{\dagger} \right) \left(D_{\mu} \phi \right) - m^{2} \phi^{\dagger} \phi = \mathcal{L}$$
(6.19)

6.5 Gauge fields

How do we construct this covariant derivative D_{μ} ? This is done by introducing an auxiliary field that can collect correction terms. Define

$$D_{\mu} = \partial_{\mu} - iA_{\mu}. \tag{6.20}$$

Here A_{μ} is the gauge field. It is also affected by the transformation,

$$(\partial_{\mu} - iA_{\mu})\phi \to \left(\partial_{\mu} - i\tilde{A}_{\mu}\right)\left(\hat{U}\phi\right)$$
 (6.21)

6.5. GAUGE FIELDS

Our task is to find how this gauge field has to transform, in order for D_{μ} to be covariant. The left hand side of (6.17) is

$$D_{\mu}\left(\hat{U}\phi\right) = \underbrace{\partial_{\mu}\left(\hat{U}\phi\right)}_{\text{use (6.16)}} - i\tilde{A}_{\mu}\left(\hat{U}\phi\right)$$
$$= \hat{U}\left[\hat{U}^{\dagger}\left(\partial_{\mu}\hat{U}\right) + \partial_{\mu}\right]\phi - i\tilde{A}_{\mu}\left(\hat{U}\phi\right)$$
$$= \hat{U}\left[\hat{U}^{\dagger}\left(\partial_{\mu}\hat{U}\right) + \partial_{\mu} - i\hat{U}^{\dagger}\tilde{A}_{\mu}\hat{U}\right]\phi \qquad (6.22)$$

The right hand side is

$$\hat{U}(D_{\mu}\phi) = \hat{U}(\partial_{\mu} - iA_{\mu})\phi \qquad (6.23)$$

So, the equality will only hold if

$$A_{\mu} \to \tilde{A}_{\mu} = \hat{U}A_{\mu}\hat{U}^{\dagger} + i\hat{U}\left(\partial_{\mu}\hat{U}^{\dagger}\right)$$
(6.24)

Let's check this, starting from the expression between square brackets in (6.22):

$$\hat{U}^{\dagger} \left(\partial_{\mu} \hat{U} \right) + \partial_{\mu} - i \hat{U}^{\dagger} \tilde{A}_{\mu} \hat{U}$$

$$= \hat{U}^{\dagger} \left(\partial_{\mu} \hat{U} \right) + \partial_{\mu} - i \hat{U}^{\dagger} \left[\hat{U} A_{\mu} \hat{U}^{\dagger} + i \hat{U} \left(\partial_{\mu} \hat{U}^{\dagger} \right) \right] \hat{U}$$

$$= \hat{U}^{\dagger} \left(\partial_{\mu} \hat{U} \right) + \partial_{\mu} - i \hat{U}^{\dagger} \hat{U} A_{\mu} \hat{U}^{\dagger} \hat{U} + \hat{U}^{\dagger} \hat{U} \left(\partial_{\mu} \hat{U}^{\dagger} \right) \hat{U}$$

$$= \partial_{\mu} - i A_{\mu} + \hat{U}^{\dagger} \left(\partial_{\mu} \hat{U} \right) + \left(\partial_{\mu} \hat{U}^{\dagger} \right) \hat{U}$$

$$= \partial_{\mu} - i A_{\mu} + \partial_{\mu} \left(\hat{U}^{\dagger} \hat{U} \right)$$

$$= \partial_{\mu} - i A_{\mu}.$$
(6.25)

It works out. So, we get to the main point of gauge theories:

Imposing local gauge invariance implies that

$$\partial_{\mu}$$
 is replaced by a covariant derivative $\partial_{\mu} - iA_{\mu}$
where the gauge field A_{μ} transforms according to
 $A_{\mu} \rightarrow \tilde{A}_{\mu} = \hat{U}A_{\mu}\hat{U}^{\dagger} + i\hat{U}\left(\partial_{\mu}\hat{U}^{\dagger}\right)$

$$(6.26)$$

The Lagrangian becomes

$$\mathcal{L} = (\partial^{\mu} - iA^{\mu}) \phi^{\dagger} (\partial_{\mu} - iA_{\mu}) \phi - m^{2} \phi^{\dagger} \phi$$
(6.27)

REMARK – We focused in our example on a U(1) local gauge symmetry, in which there is only one continuous parameter (and one generator) in the group. We got the vector potential A^{μ} from electromagnetism as a result. What if we look not at scalars, but multicomponent fields, and impose for example SU(2) local gauge invariance? Now there are three continuous parameters, or "phase angles" to turn, since every element in SU(2) can be written with the generators as

$$\hat{U} \in SU(2) \Rightarrow \exists \theta_1, \theta_2, \theta_3 : \hat{U} = \exp\left\{i\frac{\sigma_x}{2}\theta_1 + i\frac{\sigma_y}{2}\theta_1 + i\frac{\sigma_z}{2}\theta_3\right\}$$
(6.28)

with $\sigma_x, \sigma_y, \sigma_z$ the Pauli matrices. We'll need three gauge fields, indeed just as many as there are generators for the group. The electroweak theory has SU(2)local gauge invariance, and its three gauge fields give rise to the W^+, W^- and Z^0 massive vector bosons that mediate the weak nuclear force. How about SU(3)for mixing up the components of three-component fields (say, three colours of quark)? That also works, and since SU(3) has eight generators, we'll need eight gauge fields. These give rise to the eight types of gluons that mediate the strong nuclear force. You see how requiring a certain symmetry already tells you much about how many types of particles and what kind of particles to expect in the underlying Lagrangian.

This works not only in particle physics (we still need to see the link between fields and elementary particles), but it also works for general relativity. Requiring that Lorentz invariance holds locally everywhere in curved spaces forces you to change from the partial derivative to the covariant derivative $D_{\mu}u_{v} = \partial_{\mu}u_{v} + \Gamma^{\lambda}_{\mu\nu}u_{\lambda}$ where Γ is the cristoffel symbol.

6.6 The field strength

Hold on. We have introduced a new field, but we're still looking for the most general form of a Lagrangian obeying our required symmetries and having no more than second powers in the fields and their derivatives. Can't we have other terms envolving A_{μ} in our Lagrangian? Yes you can ! It gets pretty difficult once you consider $SU(2), SU(3), \dots$ let's work out what happens in U(1). This has been the example we started with in this section anyway, for which simply

$$\hat{U}\phi = e^{i\theta}\phi \tag{6.29}$$

with the phase angle θ a (position dependent) scalar. Then the gauge field transforms as

$$A_{\mu} \to \tilde{A}_{\mu} = e^{i\theta} A_{\mu} e^{-i\theta} + i e^{i\theta} \left(\partial_{\mu} e^{-i\theta} \right)$$

= $A_{\mu} + \partial_{\mu} \theta$ (6.30)

The derivative of the gauge field transforms as

$$\partial_{\nu}A_{\mu} \to \partial_{\nu}A_{\mu} + \partial_{\nu}\partial_{\mu}\theta \tag{6.31}$$

Note that a U(1) gauge transform is like adding a gradient of some scalar to the gauge vector field. Does that sound familiar? Yes, it is precisely the kind of

freedom you have for the electromagnetic vector potential. Also there you saw that the vector potential is defined "up to a gauge transform" (you have to be a bit careful here, we're working in the covariant version of Maxwell's formalism).

So how about these extra terms that would also be gauge invariant? Yang and Mills worked by trial and error. If we look at a derivative, we can see that the combination

$$F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu} \tag{6.32}$$

obeys local gauge invariace, since $\partial_{\nu}\partial_{\mu}\theta - \partial_{\mu}\partial_{\nu}\theta = 0$. But the Lagrangian is a scalar, so we need to either contract this tensor with the metric, or with itself. The latter choice brings us to

$$\mathcal{L} = (\partial^{\mu} + iA^{\mu})\phi^{\dagger}(\partial_{\mu} - iA_{\mu})\phi - m^{2}\phi^{\dagger}\phi - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}.$$
(6.33)

Where we added the 1/4 factor from convention. The tensor field $F_{\mu\nu}$ is called the *field strength* of the gauge field. If you remember the covariant version of electromagnetism, then you will immediately recognise that this field strength is the electromagnetic field tensor containing electric and magnetic fields! If you don't remember that, do not worry, you will learn this from the exercises. The Lagrangian we have obtained is the Lagrangian of the electromagnetic field (expressed through the vector potential) in interaction with a scalar complex field. As we'll see later, the "quantum" of the scalar complex field is a charged scalar boson.

6.7 Non-abelian gauge theories

The construction of the field strength in general is very complicated and requires more differential geometry. It turns out that the stuff we found for U(1)generalizes quite nicely, and the field strength in general is given by

$$F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu} - i\left[A_{\mu}, A_{\nu}\right]$$
(6.34)

where $[A_{\mu}, A_{v}] = A_{\mu}A_{v} - A_{v}A_{\mu}$ is the commutator of the gauge fields. For U(1), the components of the electromagnetic 4-vector potential commute amongst themselves, so we have nothing to worry about, we have a so-called *abelian* gauge theory. However, not all object commute: think of the components of the angular momentum operator for example. If our gauge fields contains these sorts of derivatives, then the commutator doesn't vanish, and we have a *non-abelian* gauge theory.

As a final point on gauge theories, I want to note that the field strength transforms in general as $F_{\mu\nu} \rightarrow \tilde{F}_{\mu\nu} = \hat{U}F_{\mu\nu}\hat{U}^{\dagger}$, so in the case of U(1) the field strength is invariant.

for the classical physicist:	
usual Maxwell field theory	

And God said: $\begin{cases} \boldsymbol{\nabla} \cdot \boldsymbol{\varepsilon} \mathbf{E} = \rho \\ \boldsymbol{\nabla} \cdot \mathbf{B} = 0 \\ \boldsymbol{\nabla} \times \mathbf{E} = -\partial \mathbf{B} / \partial t \\ \boldsymbol{\nabla} \times \mathbf{B} = \mu \mathbf{J} + \boldsymbol{\varepsilon} \mu \partial \mathbf{E} / \partial t \\ \mathbf{and then there was light} \end{cases}$ for the quantum field theorist: Maxwell through a gauge field

 $\begin{array}{c|c} & \text{And God said:} \\ & \psi \rightarrow \psi e^{i\theta(x)} \\ & \text{and then there was light.} \end{array}$

Bumper stickers based on Genesis 1:3

Part III Quantum fields

Chapter 7

Quantizing fields with path integrals

7.1 From classical to quantum field

The Lagrangian theory of classical fields can be seen as the extension of analytical mechanics to large numbers of coordinates $q_1, q_2, \ldots, q_j, \ldots$ interacting locally with one another. We used this to go from a chain of masses, linked with springs, to a field $\varphi(x,t)$ where x indexes which mass point you look at, and t tracks it in time. To see what the quantum version of this becomes, let's first look at the quantum version for a single of those mass points. Pick any you like, for example q_3 , and let's treat it as if it is a single particle in some external potential. We can then find the solution $\overline{q}_3(t)$ to the Euler-Lagrange equation of motion for this mass point. This $\overline{q}_3(t)$ tells you how the height of the spring varies in time, at position x = 3. The solution $\overline{q}_3(t)$ is illustrated as a thick black curve in figure 7.1: the classical trajectory of q_3 .

Quantum mechanically, there is more to reality than simply the classical trajectory. As you know from the double-slit experiment, you need to take into account all possible paths going from the initial position to the final position, and sum up the amplitudes corresponding to these paths. That is the only way you get interference, even for a single particle crossing the double-slit screen. You may imagine adding more slits or holes, and adding more screens. Taking the limit of infinitely many screens, with infinitely many holes drilled in them, is just free space, but still the quantum interference must hold. This forces an important conclusion on us: all paths $q_3(t)$ matter, not just the classical trajectory $\overline{q}_3(t)$. In the classical limit, only paths fluctuating closely near $\overline{q}_3(t)$ will give appreciable contributions to the total sum over all paths – some of these fluctuating paths are indicated in figure 7.1 as thin green curves. Looking at a particular fixed time between start and stop, these fluctuating paths will give rise to a distribution of values, that we can relate the wave function of the particle, originally located in the initial point. Also this is in contrast to the



Figure 7.1: Classically, a particle follows a unique trajectory. Quantum mechanics (as seen from the double-slit experiment) tells us that we must take into account all possible paths that go from start to finish. The possible paths can be characterized at any time slicing δ by listing the numbers $\{q_3(t_1), q_3(t_2), \ldots\}$, and taking the limit for finer slices $\delta \to 0$.

classical point of view, where there is only a single position that the particle can be at any given time.

To set up the quantum mechanics of a single particle, we need to specify (1) how to sum over all paths, and (2) the weight of a given path $q_3(t)$. Let's first tackle the question of how to sum over all paths. To do this, we will use the mental image of putting more and more screens for the particle to go through – this corresponds to slicing the time into small time steps δ . The total time interval is then reduced to $N = T/\delta$ individual snapshots, like frames in a movie. Any path from $q_3(0) = a$ to $q_3(T) = b$ is characterized by the list of positions $q_3(t_1), q_3(t_2), \ldots, q_3(t_{N-1})$ where $t_j = j\delta$. Only the first $q_3(t_0) = a$ and the last $q_3(t_N) = b$ are fixed, they are the initial and the final positions, all the others can take any value they want. Summing over all paths then becomes integrating over all values that $q_3(t_1)$ can take (in our example, real values from $-\infty$ to $+\infty$), and idem for $q_3(t_2)$, etc. As you know when you increase the frame rate of a movie, the motion seems nicer and smoother, and also here we take the limit $\delta \to 0$ (or correspondingly, $N \to \infty$):

$$\sum_{\text{paths}} \to \lim_{N \to \infty} \int_{-\infty}^{+\infty} dq_{3,1} \int_{-\infty}^{+\infty} dq_{3,1} \dots \int_{-\infty}^{+\infty} dq_{3,N-1} = \lim_{N \to 0} \prod_{j=1}^{N-1} \int_{-\infty}^{+\infty} dq_{3,j}$$
(7.1)

Here, we introduced the notation $q_{3,j}$ for $q_3(t_j)$. We also introduce a better symbol than \sum_{paths} , to emphasize that the path sum in the limit of $\delta \to 0$

becomes a path integral,

$$\int \mathcal{D}q_3 \tag{7.2}$$

We can add upper and lower bounds to the integral signs, to indicate the initial point $q_3(t=0)$ and the final point $q_3(t=T)$, if we only consider paths connecting these two spacetime points. What weight should we give a certain path? It should be a phase (to allow interference) and chosen such that in the classical limit ($\hbar \rightarrow 0$), the classical Lagrangian mechanics appears again. Feynman postulates that the action functional divided by \hbar is the phase associated with a path. So, the amplitude of a given path is

$$\exp\left\{\frac{i}{\hbar}S[q_3(t)]\right\} = \exp\left\{\frac{i}{\hbar}\int_0^T L\left(q_3, \dot{q}_3\right)dt\right\}$$
(7.3)

This fulfills the purpose: when \hbar becomes very small, the phases of nearby paths $q_3(t)$ and $q_3(t) + \delta q_3(t)$ oscillate strongly and interfere destructively, unless $\delta S = 0$ This happens only for the classical path $\overline{q}_3(t)$. So, the amplitude to go from spacetime point q_a, t_a to q_b, t_b is the sum of this path amplitude over all paths:

$$\int_{q_3(0)=a}^{q_3(T)=b} \mathcal{D}q_3 \exp\left\{\frac{i}{\hbar}S[q_3(t)]\right\}$$
(7.4)

To be complete, I must note that I have swept something under the rug: the normalization factors, i.e. the measure of the N-fold integral as we take the limit $N \to \infty$ is not trivial. Just like we had to be careful when taking the limit in space – reducing the mass of each point, and strengthing the spring constant each time we halve the distance between q_j and q_{j+1} , we also have to be careful when taking the limit in times. However, the cases when we need to worry about this weight are rare, and we won't cover this topic in this course.

Let's go now from a single mass point to the field, as in figure 7.2. In our example of the string of mass points connected by springs, we want to see how the string as a whole moves and wobbles as a function of time. That is precisely what classical field theory tells us. The solution $\bar{\varphi}(x,t)$ the classical field equations provides information on the height of the string at position x, and at time t. It is clear that this classical solutions associates a single value to each spacetime point. Again this changes when quantum mechanics is brought into the picture: now for each mass element of the string we have to look at all possible paths – and this in turn means that we now have to look at all possible realizations of the field $\varphi(x,t)$, and not restrict ourselves to that one realization that solves the classical field equation. Of course, fields that represent fluctuations around the classical result will contribute most strongly. As illustrated in figure 7.3, in each spacetime point we have to consider a distribution of possible values, generated by the fluctuating field.



Figure 7.2: Remember how we constructed the classical field as a string of particles – the index of the generalized coordinate q_j is now interpreted as a position in space.



Figure 7.3: For each mass point in the string we now have to look at all possible paths from initial to final position. This means that for the field $\varphi(x, t)$ representing the height of the string in spacetime, we get a distribution of values in each spacetime point. We'll need to sum over all possible field configurations.

7.1. FROM CLASSICAL TO QUANTUM FIELD

We can now reformulate our single-particle quantization programme into a field quantization protocol. We want to find the quantum mechanical amplitude, call it Z, that the field starts in its ground state (no excitations of the string), and ends up at a later time T back in its ground state. To do this, we have to sum over all possible field realizations that start with all $q_j(t = 0)$'s equal, and ends with all $q_j(t = T)$'s equal. In between, the field can wiggle around however it wants. To find Z, again we have to figure out (1) how to sum over all possible field realizations $\varphi(x, t)$, and (2) we need to figure out the amplitude to associate with each field realization.

Summing over field realizations is rather easy to generalize from summing over paths. We have already sliced the time domain for the paths into $N = T/\delta$ steps of duration δ . We also have chopped up the string into $M = L/\varepsilon$ segments of size ε . This discretizes spacetime and allows to represent the field by a finite collection of $q_{x,t}$ values in each each point of the spacetime grid. All we need to do is to allow these $q_{x,t}$ values to take on any value, and then take the limit as δ and ε both become small:

$$\sum_{\text{field realizations}} \to \lim_{N,M\to\infty} \prod_{i=0}^{M} \prod_{j=1}^{N-1} \int_{-\infty}^{+\infty} dq_{i,j}$$
(7.5)

Two important remarks are in place here:

- First, I again emphasize that taking the limit is a tricky business. For some Langrangians, you get a lot of infinities, and you need to renormalize the parameters (as we did for the mass and the spring constant) and follow the renormalization flow, and think about the integration measure. Sometimes, it is not possible to get rid of these infinities, and the theory is not renormalizable. In that case, we cannot set up a good quantum field theory corresponding to the discretized model.
- Second, the field values are not necessary single real numbers. Sometimes they are complex numbers, and we have to integrate over the complex plane rather than the real axis in each point. Other possibilities are angular variables, and we have to integrate over $[0, 2\pi]$ and sum over winding numbers (how often does the coordinate go around). Still another possibility are vector fields, where the components get scrambled as you change your coordinate frame and it is important to choose a useful set of coordinates.

We also generalize our notation for the path-integral over field realizations, noting it as $\int \mathcal{D}\varphi$, where $\varphi(x,t)$ is the continuum version of $q_{i,j}$ as before. Since we no longer sum over paths, but over field realizations, it can be argued that "path integral" over fields is not such a good name. You can call it "functional integral" or "Feynman integral" or "field integral" if you want make this point. The amplitude of a field configuration is simply going to be

$$\exp\left\{\frac{i}{\hbar}S[\varphi]\right\} = \exp\left\{\frac{i}{\hbar}\int_{V} \mathcal{L}\left(\varphi,\partial_{\mu}\varphi\right)d^{4}x\right\},\tag{7.6}$$

where \mathcal{L} is the classical field Lagrangian, and we integrate over a block V of spacetime corresponding to the time interval T and the size of the system. Hence, the sum over all field realizations, weighed by the correct amplitude for the field, can be written as

$$Z = \int \mathcal{D}\varphi \exp\left\{\frac{i}{\hbar}S[\varphi]\right\}.$$
(7.7)

This is the generalization of the path-integral formulation of quantum mechanics, to the Lagrangian formulation of quantum field theory.

7.2 Gaussian Integral Intermezzo

7.2.1 Wick decomposition

Quantum field theory is replete with Gaussian integrals. That is partly because that type of integral is the only one with which we can get analytic solutions for Z. But even more importantly, it is also often the case that the green splotch in figure 7.3 (representing the distribution of values for the quantum field $q_{4,2}$ at x = 4, t = 2) is well approximated by a Gaussian centered around the classical value¹. So it is definitely worth having a closer look at the good old Gaussian. The basic result is

$$G = \int_{-\infty}^{+\infty} e^{-x^2/2} dx = \sqrt{2\pi}.$$
 (7.8)

It is simple to prove of this by calculating G^2 and going from cartesian to polar coordinates

$$G^{2} = \int_{-\infty-\infty}^{+\infty+\infty} \int_{-\infty-\infty}^{\infty} e^{-(x^{2}+y^{2})/2} dx dy$$
$$= \int_{0}^{2\pi} d\theta \int_{0}^{\infty} e^{-r^{2}/2} r dr = -2\pi \left. e^{-r^{2}/2} \right|_{0}^{\infty} = 2\pi$$
(7.9)

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¹This is the "field version" of Gaussian wave packets for moving atoms. Very often the wave function of some particle can be thought of as a gaussian wave packet centered around the position of that particle in the classical trajectory. The width of that wave packet is Δx , the quantum uncertainty on the particle's position.

7.2. GAUSSIAN INTEGRAL INTERMEZZO

A simple substitution generalizes this to

$$\int_{-\infty}^{+\infty} e^{-ax^2/2} dx = \sqrt{\frac{2\pi}{a}}$$
(7.10)

From this, we get a bunch of other integrals using a clever trick. Since

$$-2\frac{d}{da}e^{-ax^2/2} = x^2e^{-ax^2/2} \tag{7.11}$$

we get

$$\int_{-\infty}^{+\infty} x^2 e^{-ax^2/2} dx = -2\frac{d}{da} \left(\sqrt{\frac{2\pi}{a}}\right) = \sqrt{2\pi} \frac{1}{a^{3/2}}$$
(7.12)

Using the Gaussian as a probability distribution, we can then calculate the expectation value $\langle x^2 \rangle$ and find

$$\langle x^2 \rangle = \frac{\int_{-\infty}^{+\infty} x^{2n} e^{-ax^2/2} dx}{\int_{-\infty}^{+\infty} e^{-ax^2/2} dx} = \frac{1}{a}$$
 (7.13)

We can repeat this derivation n times,

$$\int_{-\infty}^{+\infty} x^{2n} e^{-ax^2/2} dx = \left(-2\frac{d}{da}\right)^{2n} \left(\sqrt{\frac{2\pi}{a}}\right) = \sqrt{2\pi} \frac{1 \times 3 \times 5 \times \dots \times (2n-1)}{a^{n+1/2}}$$
(7.14)

The product in the denominator is also called a "double factorial" and noted as (2n-1)!!. It is like a factorial, but only contains the odd integers up to 2n-1. The expectation value $\langle x^{2n} \rangle$ is then given by

$$\langle x^{2n} \rangle = \frac{(2n-1)!!}{a^n}$$
 (7.15)

The double factorial is also the number of ways to connect 2n points pairwise. There are precisely (2n-1)!! ways to pair up the 2n factor is in $\langle x^{2n} \rangle = \langle x.x.x...x \rangle$. Indeed the first point one has the choice between 2n-1 others. The next one has a choice out of two less than that, 2n-3. That way you step down the integers by 2 and obtain the double factorial. This pairing up of 2n points is known as a *Wick contraction*. Per pair we get a factor $\langle x.x \rangle = 1/a$. Finally, note that products of an odd number of x's will give an integral that is zero.

The Wick decomposition rule tells you that you can obtain $\langle x^{2n} \rangle$ as a sum, over all possible ways to pair up the x's, of the product of these pairs $\langle x.x \rangle \langle x.x \rangle \dots \langle x.x \rangle = a^{-n}$.

7.2.2 Completing the squares

There's another way of obtaining the result for $\langle x^{2n} \rangle$, and that is through

$$G(J) = \int_{-\infty}^{+\infty} e^{-ax^2/2 + Jx} dx$$
(7.16)

The result can be found by completing the square,

$$-\frac{1}{2}ax^{2} + Jx = -\frac{1}{2}a\left(x - \frac{J}{a}\right) + \frac{J^{2}}{2a}$$
(7.17)

with which

$$G(J) = e^{J^2/(2a)} \int_{-\infty}^{+\infty} \exp\left\{-\frac{1}{2}a\left(x - \frac{J}{a}\right)\right\} dx$$
$$= \sqrt{\frac{2\pi}{a}} e^{J^2/(2a)}.$$
(7.18)

Now we can differentiate with respect to J in order to bring powers of x down,

$$\frac{d^{2n}G(J)}{dJ^{2n}} = \int_{-\infty}^{+\infty} x^{2n} e^{-ax^2/2 + Jx} dx$$
(7.19)

Hence, our expectation value can be written as

$$\left\langle x^{2n} \right\rangle = \frac{\int_{-\infty}^{+\infty} x^{2n} e^{-ax^2/2} dx}{\int_{-\infty}^{+\infty} e^{-ax^2/2} dx} = \sqrt{\frac{a}{2\pi}} \left. \frac{d^{2n} G(J)}{dJ^{2n}} \right|_{J \to 0}$$
(7.20)

which yields

$$\langle x^{2n} \rangle = \left(\frac{d}{dJ} \right)^{2n} \left(e^{J^2/(2a)} \right) \bigg|_{J \to 0}$$
 (7.21)

Let's do some examples:

$$\langle x^2 \rangle = \frac{d^2}{dJ^2} e^{J^2/(2a)} = \frac{d}{dJ} \left(\frac{J}{a} e^{J^2/(2a)} \right) \Big|_{J \to 0}$$
 (7.22)

$$= \left[\frac{1}{a} + \left(\frac{J}{a}\right)^{2}\right] e^{J^{2}/(2a)} \bigg|_{J \to 0} = \frac{1}{a}$$
(7.23)

Deriving with respect to J will make the expression between square brackets an ever more complicated polynomial in J:

$$\frac{d^3}{dJ^3}e^{J^2/(2a)} = \left[3\frac{J}{a^2} + \left(\frac{J}{a}\right)^3\right]e^{J^2/(2a)}$$
(7.24)

$$\frac{d^4}{dJ^4}e^{J^2/(2a)} = \left[\frac{3}{a^2} + 6\frac{J^2}{a^3} + \left(\frac{J}{a}\right)^4\right]e^{J^2/(2a)}$$
(7.25)
etc ...

The polynomials corresponding to even/odd derivatives have all even/odd powers in J. Only the even ones are nonzero in the limit $J \to 0$. We can easily read off that $\langle x^2 \rangle = 3/a^2$ in line with our previous result. For this calculation, the Jx term in the exponent is an auxiliary term, a trick to find the result, after which we let it vanish again. Now that we have taken a closer look at single gaussian integrals, it is time to tackle products of a large number of such integrals and figure out what happens when we replace a by a matrix A.

7.3 The quantized oscillating string

Let's have a closer look at our string of mass points connected by springs. We found that the Lagrangian density of this string equals

$$\mathcal{L} = \frac{1}{2} \partial_{\mu} \varphi \partial^{\mu} \varphi = \frac{1}{2} \left(\partial_{t} \varphi \right)^{2} - \frac{1}{2} \left(\partial_{x} \varphi \right)^{2}$$
(7.26)

so that the action functional is

$$S[\varphi] = \frac{1}{2} \int \left[\left(\partial_t \varphi \right)^2 - \left(\partial_x \varphi \right)^2 \right] dx \tag{7.27}$$

We are going to work in a discretized version, slicing the time T in six pieces $\delta = T/6$. Note that at initial and final times the positions are zero so $\varphi_{x,0} = 0 = \varphi_{x,6}$, so there are five moments in time, five frames in our movie. Equally, we'll segment the string in five pieces of length ε , and get five mass points x = 1, 2, 3, 4, 5. That way we have a very simple grid in our spacetime. The field realization is fully determined by 25 numbers $\varphi_{x,t}$ with $x \in \{1, 2, 3, 4, 5\}$ and $t \in \{1, 2, 3, 4, 5\}$. The derivatives become differences in our discrete spacetime, so we get for the action:

$$S\left[\varphi_{1,1},\varphi_{1,2},\dots,\varphi_{5,5}\right] = \frac{1}{2} \left[\sum_{x=1}^{5} \sum_{t=1}^{6} \left(\frac{\varphi_{x,t}-\varphi_{x,t-1}}{\delta}\right)^2 - \sum_{x=2}^{5} \sum_{t=1}^{5} \left(\frac{\varphi_{x,t}-\varphi_{x-1,t}}{\varepsilon}\right)^2\right]$$
(7.28)

Now the action takes as input all 25 numbers needed to characterize a single field configuration. With these numbers you compute a single, real number S as



Figure 7.4: In quantum field theory, all possible field configurations (of which three are shown in this figure) contribute, not just the one field configuration that satisfies the classical field equations (even though this may give the main contribution). You need a sum over all possible configurations of the corresponding phase factor, determined by the action functional. You could devise a "Monte-Carlo" approach, generating field configurations randomly and then taking terms in this sum, but without further guidance it would converge poorly... unless maybe you start from the classical solution and add some (try Gaussian) noise to each point to generate the sample.

output. The amplitude corresponding to the field configuration specified by the 25 numbers is then $\exp\{iS/\hbar\}$. Easy peasy. The vacuum-vacuum transition amplitude then is given by the sum over all field configurations of the corresponding $\exp\{iS/\hbar\}$ contributions, as illustrated in figure (7.4). We can write this as

$$Z = \left(\prod_{x=1}^{5} \prod_{t=1}^{5} \int_{-\infty}^{+\infty} d\varphi_{x,t}\right) \exp\left\{\frac{i}{\hbar} S\left[\varphi_{1,1}, \varphi_{1,2}, \dots, \varphi_{5,5}\right]\right\}$$
(7.29)

If it suits us we could rename the 25 fields as $\varphi_1, ..., \varphi_{25}$ rather than keep separate space and time label, that way we can write

$$Z = \int_{-\infty}^{+\infty} d\varphi_1 \dots \int_{-\infty}^{+\infty} d\varphi_{25} \exp\left\{\frac{i}{\hbar} S\left[\varphi_1, \dots, \varphi_{25}\right]\right\}$$
(7.30)

You see moreover that the action is *quadratic* in the field variables. This allows us to write the action compactly as a multivariate Gaussian integral:

$$Z = \int_{-\infty}^{+\infty} d\varphi_1 \dots \int_{-\infty}^{+\infty} d\varphi_{25} \exp\left\{-\frac{1}{2} \sum_{j=1}^{25} \sum_{\ell=1}^{25} \varphi_j A_{j\ell} \varphi_\ell\right\}$$
(7.31)

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Most of the 25×25 elements of A will be empty, only rows and columns corresponding to $\varphi_{x,t}$'s adjacent in space or time will contain values. In other words, $\varphi_{x,t}$ couples to $\varphi_{x,t+1}, \varphi_{x,t-1}$ and to $\varphi_{x+1,t}, \varphi_{x-1,t}$, and these are the only four elements in the row corresponding to $\varphi_{x,t}$ which are non-zero, all 21 other entries of that row of A are zero's. We say that A is a sparse matrix. We can also choose the matrix to be symmetric. In the action functional we have terms that go like $(\varphi_{15} - \varphi_{16})^2 = \varphi_{15}^2 - 2\varphi_{15}\varphi_{16} + \varphi_{16}^2$. The coefficients of the squares φ_{15}^2 go on the diagonal of A, namely $A_{15,15}$. The coefficient of the double product term $\varphi_{15}\varphi_{16}$ can be placed entirely in $A_{15,16}$, or we can put half of it in $A_{15,16}$ and the other half in $A_{16,15}$. We'll choose this symmetric way of defining A because every symmetric matrix is, up to choice of an orthonormal basis, a diagonal matrix. And hence we get

$$Z = \sqrt{2\pi^{25}} \frac{1}{\sqrt{\det(A)}}$$
(7.32)

where det (A) is the determinant of A. It's obvious that this is the generalization of the Gaussian integral (7.10) where now a is a matrix A.

Let's proove this result. Collecting all the φ_{ℓ} in a column vector φ , we can rewrite (7.31) as

$$Z = \int_{-\infty}^{+\infty} d\varphi_1 \dots \int_{-\infty}^{+\infty} d\varphi_{25} \exp\left\{-\varphi^T \cdot A \cdot \varphi\right\}$$
(7.33)

Any real symmetric matrix can be diagonalized: three exists an special orthogonal matrix O such that $O \cdot A \cdot O^T = \tilde{A}$ is diagonal, $\tilde{A}_{jk} = \lambda_j \delta_{jk}$. Orthogonality means that $O^T \cdot O = 1$ is the unit matrix. Hence,

$$\varphi^{T} \cdot A \cdot \varphi = \varphi^{T} \cdot (O^{T} \cdot O) \cdot A \cdot (O^{T} \cdot O) \cdot \varphi$$
$$= (\varphi^{T} \cdot O^{T}) \cdot O \cdot A \cdot O^{T} \cdot (O \cdot \varphi)$$
$$= \chi^{T} \cdot \tilde{A} \cdot \chi$$
(7.34)

Here, $\boldsymbol{\chi} = O \cdot \boldsymbol{\varphi}$ is again a column containing 25 new variables, and we'll use them as the new integration variables. The Jacobian of the orthogonal transformation is one, and if all φ_j 's can range from $-\infty$ to $+\infty$, so can all χ_j . Hence

$$Z = \int_{-\infty}^{+\infty} d\chi_1 \dots \int_{-\infty}^{+\infty} d\chi_{25} \exp\left\{-\sum_{j=1}^{25} \lambda_j \chi_j^2\right\}.$$
 (7.35)

Here the λ_j 's are the eigenvalues of the matrix A. Now each integral can be done separately,

$$Z = \prod_{j=1}^{25} \left(\int_{-\infty}^{+\infty} \exp e^{-\lambda_j \chi_j^2} d\chi_j \right) = \prod_{j=1}^{25} \sqrt{\frac{2\pi}{\lambda_j}}$$
(7.36)

Since det $(A) = \prod_{j=1}^{25} \lambda_j$, this proves (7.32).

Again, two important remarks:

• First, I come back to my point about the integration measure that I swept under the rug in expression (7.5). You see a silly factor $(2\pi)^{25/2}$ appearing, where the 25 comes from the 5×5 spacetime points. As we take more and more spacetime points, a finer grid, this diverges. We would not have this problem if we'd written

$$\sum_{\text{field realizations}} \to \lim_{N,M\to\infty} \prod_{i=0}^{M} \prod_{j=1}^{N-1} \int_{-\infty}^{+\infty} \frac{dq_{i,j}}{\sqrt{2\pi}}$$

in stead of (7.5). Having done the calculation, we a posteriori infer that this is the correct way of summing over all field realizations, resulting in $Z = 1/\sqrt{\det(A)}$. However, this integration measure should not worry us too much: factors such as $(2\pi)^{25/2}$ will drop out when calculating expectation values, as you will see!

• Second, this results holds for real scalar fields. Later on, we'll introduce another denizen of spacetime, the Grassmann variables, and for those the result will be different. But also for complex fields ϕ or angular variables or other beasts, it is different. Let's look at the case of complex scalar fields ϕ . There we must integrate for each ϕ_j over the complex plane, rather than over the real axis. Hence we get for our 5×5 grid:

$$\sum_{\text{field realizations}} \to \prod_{j=1}^{25} \int_{-\infty}^{+\infty} \frac{d\phi_{R,j}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{d\phi_{I,j}}{\sqrt{2\pi}}, \qquad (7.37)$$

where $\phi_{R,j}$ and $\phi_{I,j}$ represent real and imaginary parts of ϕ_j . Now the matrix A can be chosen hermitian, so that it can be diagonalized by a unitary matrix, and we need to do integrals of the type

$$\int_{-\infty}^{+\infty} \frac{d\phi_{R,j}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{d\phi_{I,j}}{\sqrt{2\pi}} e^{-\lambda_j \phi_j^* \phi_j} = \int_{-\infty}^{+\infty} \frac{d\phi_{R,j}}{\sqrt{2\pi}} e^{-\lambda_j \phi_{R,j}^2} \int_{-\infty}^{+\infty} \frac{d\phi_{I,j}}{\sqrt{2\pi}} e^{-\lambda_j \phi_{I,j}^2} = \frac{1}{\lambda_j}.$$
(7.38)

From this we can conclude that for complex scalar fields,

$$Z = \frac{1}{\det\left(A\right)}.\tag{7.39}$$
7.4 Expectation values

7.4.1 Source terms

Also in (7.31) we can add source terms, and investigate

$$Z_{J} = \int_{-\infty}^{+\infty} d\varphi_{1} \dots \int_{-\infty}^{+\infty} d\varphi_{25} \exp\left\{-\frac{1}{2} \sum_{j=1}^{25} \sum_{\ell=1}^{25} \varphi_{j} A_{j\ell} \varphi_{\ell} + \sum_{\ell=1}^{25} J_{\ell} \varphi_{\ell}\right\}$$
(7.40)

In our model of the string as a set of mass points connected with springs, an extra term $J_{x,t}\varphi_{x,t}$ corresponds to a force kick at position x and time t, as illustrated in figure 7.5 Without such kicks, the system may just remain in its ground state. The kick will disturb that vacuum, and be a source of propagating waves, like a stone thrown in a pool is the source of propagating ripples.



Figure 7.5: Pushing or pulling on the mass point labeled q_4 of the springy string corresponds to adding a term $J_4(t)q_4$ to the potential energy in the Lagrangian.

To solve this, we again resort to diagonalization of the matrix A by an orthogonal matrix O. This time we must also introduce the row vector \mathbf{J} containing the values J_{ℓ} , so that we can write (7.40) as

$$Z_J = \int_{-\infty}^{+\infty} d\varphi_1 \dots \int_{-\infty}^{+\infty} d\varphi_{25} \exp\left\{-\varphi^T \cdot A \cdot \varphi + \mathbf{J} \cdot \varphi\right\}$$
(7.41)

The diagonalisation happens as in (7.34), but we also have to include

$$\mathbf{J} \cdot \boldsymbol{\varphi} = \mathbf{J} \cdot (O^T \cdot O) \cdot \boldsymbol{\varphi} = (\mathbf{J} \cdot O^T) \cdot (O \cdot \boldsymbol{\varphi}) = \mathbf{\bar{J}} \cdot \boldsymbol{\chi}$$
(7.42)

with $\overline{\mathbf{J}} = \mathbf{J} \cdot O^T$, having components

$$\bar{J}_k = \sum_{\ell} J_\ell O_{\ell k}^T = \sum_{\ell} O_{k\ell} J_\ell \tag{7.43}$$

Then

$$Z_{J} = \int_{-\infty}^{+\infty} d\chi_{1} \dots \int_{-\infty}^{+\infty} d\chi_{25} \exp\left\{-\sum_{j=1}^{25} \lambda_{j} \chi_{j}^{2} + \sum_{j=1}^{25} \bar{J}_{j} \chi_{j}\right\}$$
(7.44)

$$= \prod_{j=1}^{25} \left(\int_{-\infty}^{\infty} d\chi_j \exp\left\{ -\lambda_j \chi_j^2 + \bar{J}_j \chi_j \right\} \right)$$
(7.45)

Using (7.18) we find

$$Z_J = \prod_{j=1}^{25} \sqrt{\frac{2\pi}{\lambda_j}} \exp\left\{\bar{J}_j \frac{1}{2\lambda_j} \bar{J}_j\right\}$$
$$= \frac{\sqrt{2\pi}^{25}}{\det(A)} \exp\left\{\sum_{j=1}^{25} \bar{J}_j \frac{1}{2\lambda_j} \bar{J}_j\right\}$$
(7.46)

Note that

$$\frac{1}{2}\mathbf{J}\cdot A^{-1}\cdot\mathbf{J} = \frac{1}{2}\mathbf{J}\cdot\left(O^{T}\cdot O\right)\cdot A^{-1}\cdot\left(O^{T}\cdot O\right)\cdot\mathbf{J} = \sum_{j=1}^{25}\bar{J}_{j}\frac{1}{2\lambda_{j}}\bar{J}_{j}.$$
 (7.47)

Hence we find

$$Z_J = \frac{\sqrt{2\pi}^{25}}{\sqrt{\det(A)}} \exp\left\{\frac{1}{2} \sum_{k,\ell=1}^{25} J_k A_{kl}^{-1} J_\ell\right\}$$
(7.48)

7.4.2 Correlations

Now we can look at expectation values $\langle \varphi_i \varphi_j \rangle$. If the fluctuations of field at the spacetime point *i* are uncorrelated with the fluctuations at spacetime point *j*, then this expectation value is zero. However, in general what happens at one spacetime point influences the field in other spacetime points as well. Experiments typically probe such correlations: disturbing the field at one point and measuring the effect at another point. The expectation value is given by

$$\left\langle \varphi_{i}\varphi_{j}\right\rangle = \frac{\int_{-\infty}^{+\infty} d\varphi_{1}\dots\int_{-\infty}^{+\infty} d\varphi_{25} \varphi_{i}\varphi_{j} \exp\left\{-\frac{1}{2}\sum_{k,\ell=1}^{25} \varphi_{k}A_{k\ell}\varphi_{\ell}\right\}}{\int_{-\infty}^{+\infty} d\varphi_{1}\dots\int_{-\infty}^{+\infty} d\varphi_{25} \exp\left\{-\frac{1}{2}\sum_{k,\ell=1}^{25} \varphi_{k}A_{k\ell}\varphi_{\ell}\right\}}$$
(7.49)

We already know the denominator, so

$$\left\langle \varphi_i \varphi_j \right\rangle = \sqrt{\frac{\det(A)}{(2\pi)^{25}}} \int_{-\infty}^{+\infty} d\varphi_1 \dots \int_{-\infty}^{+\infty} d\varphi_{25} \ \varphi_i \varphi_j \exp\left\{-\frac{1}{2} \sum_{k,\ell=1}^{25} \varphi_k A_{k\ell} \varphi_\ell\right\}$$
(7.50)

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7.4. EXPECTATION VALUES

Now, the trick with (7.18) will come in handy! Indeed,

$$\langle \varphi_i \varphi_j \rangle = \sqrt{\frac{\det(A)}{(2\pi)^{25}}} \frac{d}{dJ_i} \frac{d}{dJ_j} \left[\int_{-\infty}^{+\infty} d\varphi_1 \dots \int_{-\infty}^{+\infty} d\varphi_{25} \right]$$
(7.51)

$$\exp\left\{-\frac{1}{2}\sum_{k,\ell=1}^{25}\varphi_k A_{k\ell}\varphi_\ell + \sum_{\ell=1}^{25}J_\ell\varphi_\ell\right\}\right]_{\mathbf{J}=0}$$
(7.52)

We know the result for the integral, and find

$$\left\langle \varphi_i \varphi_j \right\rangle = \left. \frac{d}{dJ_i} \frac{d}{dJ_j} \exp\left\{ \frac{1}{2} \sum_{k,\ell=1}^{25} J_k A_{kl}^{-1} J_\ell \right\} \right|_{\mathbf{J}=0}.$$
 (7.53)

This is the generalization of expression (7.21) to the multivariate case.

Let's work this out for a specific example, $\langle \varphi_7 \varphi_8 \rangle$, to see how this works. First, we derive with respect to J_7 ,

$$\frac{d}{dJ_7} \exp\left\{\frac{1}{2} \sum_{k,\ell=1}^{25} J_k A_{kl}^{-1} J_\ell\right\}$$
(7.54)

In this double sum, J_7 appears in terms with k = 7 or $\ell = 7$. Hence, we get for the derivative

$$\frac{1}{2} \left(\sum_{\ell=1}^{25} A_{7\ell}^{-1} J_{\ell} + \sum_{k=1}^{25} J_k A_{k7}^{-1} \right) \exp\left\{ \frac{1}{2} \sum_{m,n=1}^{25} J_m A_{mn}^{-1} J_n \right\}.$$
 (7.55)

Deriving this with respect to J_8 , we get contributions from the piece between round brackets, and contributions from deriving the exponent again. Hence, we have

$$\frac{d}{dJ_8} \frac{d}{dJ_7} \exp\left\{\frac{1}{2} \sum_{k,\ell=1}^{25} J_k A_{kl}^{-1} J_\ell\right\}$$

$$= \left[\frac{1}{2} \left(A_{78}^{-1} + A_{87}^{-1}\right) + \frac{1}{4} \left(\sum_{\ell=1}^{25} A_{7\ell}^{-1} J_\ell + \sum_{k=1}^{25} J_k A_{k7}^{-1}\right) \times \left(\sum_{\ell'=1}^{25} A_{8\ell'}^{-1} J_{\ell'} + \sum_{k'=1}^{25} J_{k'} A_{k'8}^{-1}\right)\right] \exp\left\{\frac{1}{2} \sum_{m,n=1}^{25} J_m A_{mn}^{-1} J_n\right\} (7.56)$$

Putting J = 0 in this expression, we find

$$\langle \varphi_7 \varphi_8 \rangle = \frac{1}{2} \left(A_{78}^{-1} + A_{87}^{-1} \right) = A_{78}^{-1}$$
 (7.57)

where the last equality holds since A^{-1} is symmetric.

7.4.3 Higher order correlations

Now we have our basic building block for the Wick decomposition, namely the expectation value for a *pair* of field variables, $\langle \varphi_i \varphi_j \rangle = A_{ij}^{-1}$. With a lot of ambition, we will now calculate $\langle \varphi_8 \varphi_7 \varphi_4 \varphi_3 \rangle$. Use the symmetry of A^{-1} , and start the derivations. First derive with respect to J_8 :

$$\frac{d}{dJ_8} \to \left(\sum_{\ell} A_{8\ell}^{-1} J_\ell\right) e^{\frac{1}{2} \mathbf{J} A^{-1} \mathbf{J}}.$$
(7.58)

Then, with J_7 :

$$\underset{d/(dJ_7)}{\rightarrow} \left[A_{87}^{-1} + \left(\sum_{\ell} A_{8\ell}^{-1} J_{\ell} \right) \left(\sum_{k} A_{7k}^{-1} J_{k} \right) \right] e^{\frac{1}{2} \mathbf{J} A^{-1} \mathbf{J}}$$
(7.59)

Next, with J_4 :

$$\stackrel{\longrightarrow}{}_{d/(dJ_4)} \left[A_{84}^{-1} \left(\sum_k A_{7k}^{-1} J_k \right) + \left(\sum_\ell A_{8\ell}^{-1} J_\ell \right) A_{74}^{-1} + A_{87}^{-1} \left(\sum_m A_{4k}^{-1} J_k \right) \right. \\ \left. \left(\sum_\ell A_{8\ell}^{-1} J_\ell \right) \left(\sum_k A_{7k}^{-1} J_k \right) \left(\sum_m A_{4k}^{-1} J_k \right) \right] e^{\frac{1}{2} \mathbf{J} A^{-1} \mathbf{J}}$$
(7.60)

Finally, with J_3 :

$$\stackrel{\rightarrow}{\underset{d/(dJ_3)}{\longrightarrow}} \left[A_{84}^{-1} A_{73}^{-1} + A_{83}^{-1} A_{74}^{-1} + A_{87}^{-1} A_{43}^{-1} + A_{83}^{-1} \left(\sum_{k} A_{7k}^{-1} J_{k} \right) \left(\sum_{m} A_{4k}^{-1} J_{k} \right) + \left(\sum_{\ell} A_{8\ell}^{-1} J_{\ell} \right) A_{73}^{-1} \left(\sum_{m} A_{4k}^{-1} J_{k} \right) + \left(\sum_{\ell} A_{8\ell}^{-1} J_{\ell} \right) \left(\sum_{k} A_{7k}^{-1} J_{k} \right) A_{43}^{-1} \\ + \left(\sum_{\ell} A_{8\ell}^{-1} J_{\ell} \right) \left(\sum_{k} A_{7k}^{-1} J_{k} \right) \left(\sum_{m} A_{4m}^{-1} J_{m} \right) \left(\sum_{n} A_{3n}^{-1} J_{n} \right) \right] e^{\frac{1}{2} \mathbf{J} A^{-1} \mathbf{J}}$$

Putting $\mathbf{J} = 0$ in this gives

$$\langle \varphi_8 \varphi_7 \varphi_4 \varphi_3 \rangle = A_{84}^{-1} A_{73}^{-1} + A_{83}^{-1} A_{74}^{-1} + A_{87}^{-1} A_{43}^{-1}$$
(7.61)

Note that this is equal to

$$\langle \varphi_8 \varphi_7 \varphi_4 \varphi_3 \rangle = \langle \varphi_8 \varphi_7 \rangle \langle \varphi_4 \varphi_3 \rangle + \langle \varphi_8 \varphi_4 \rangle \langle \varphi_7 \varphi_3 \rangle + \langle \varphi_8 \varphi_3 \rangle \langle \varphi_7 \varphi_4 \rangle \tag{7.62}$$

It was the brilliant insight of Wick to see the pattern emerging in the calculation. In order to calculate the expectation value of products like $\langle \varphi_{14}\varphi_{11}\varphi_8\varphi_7\varphi_4\varphi_3\rangle$, you first need to list all the ways of making pairs. These are called Wick contractions. For each Wick contraction, you calculate the product of the expectation values of the pairs. And then you sum over all Wick contractions:

$$\langle \varphi_i \varphi_j \dots \varphi_k \varphi_\ell \rangle = \sum_{\text{Wick contractions}} A_{ab}^{-1} \dots A_{cd}^{-1}$$
 (7.63)

We come back to our two remarks. First, note that the nasty factors of $(2\pi)^{25/2}$ dropped out of the calculation, as they appear both in the numerator and the denominator of (7.49). So, all this business of worrying about the integration measure is not really necessary when we calculate these expectation values. Second, although the result here also holds for complex fields, for other denizens of spacetime we need to thread more carefully.

7.5 Continuum limit

Let's summarize the results in the continuum limit. We saw that the vacuum-tovacuum expectation value Z is given by a sum over all spacetime configurations of the field (that start and end in vacuum), weighed by a phase factor where the action (in units of \hbar) is the phase:

$$Z = \int \mathcal{D}\varphi \exp\left\{\frac{i}{\hbar}S[\varphi]\right\}$$
(7.64)

A general quadratic action functional of the field can be written as

$$\frac{i}{\hbar}S = -\frac{1}{2}\int dx \int dy \,\varphi_x A_{xy}\varphi_y + \int dx \,J_x\varphi_x \tag{7.65}$$

$$\Rightarrow \quad Z(J) = \int \mathcal{D}\varphi \exp\left\{-\frac{1}{2}\int dx \int dy \ \varphi_x A_{xy}\varphi_y + \int dx J_x \varphi_x\right\} (7.66)$$

where x, y are *spacetime* points (and we integrate over both space and time components). We found

$$Z(J) = \frac{1}{\sqrt{\det(A)}} \exp\left\{\frac{1}{2} \int dx \int dy \ J_x A_{xy}^{-1} J_y\right\}$$
(7.67)

Remember that the equality holds when we use the correct integration measure for $\int \mathcal{D}\phi$, it is safer to write a proportionality here. To avoid this problem altogether, we write

$$Z(J) = Z(0) \exp\left\{\frac{1}{2} \int dx \int dy \ J_x A_{xy}^{-1} J_y\right\}$$
(7.68)

where Z_0 is the result for all J = 0. This allows us to calculate take expectation values of products of the fields (in spacetime points a, b) for the action without the source terms ($\mathbf{J} = 0$)

$$\langle \varphi_a \varphi_b \rangle = \frac{\int \mathcal{D}\varphi \ \varphi_a \varphi_b \exp\left\{-\frac{1}{2} \int dx \int dy \ \varphi_x A_{xy} \varphi_y\right\}}{\int \mathcal{D}\varphi \ \exp\left\{-\frac{1}{2} \int dx \int dy \ \varphi_x A_{xy} \varphi_y\right\}}$$
(7.69)

by taking (functional) derivatives with respect to J_a, J_b :

$$\langle \varphi_a \varphi_b \rangle = \frac{1}{Z(0)} \left. \frac{\delta^2 Z(J)}{\delta J_a \delta J_b} \right|_{J=0}$$

$$(7.70)$$

$$= \frac{\delta^2}{\delta J_a \delta J_b} \exp\left\{\frac{1}{2} \int dx \int dy \ J_x A_{xy}^{-1} J_y\right\} \bigg|_{J=0} = A_{ab}^{-1}.$$
 (7.71)

Expectation values for products of more fields can always be calculated from combinations of this pairwise result, by summing pairwise products over all ways of pairing (all Wick contractions):

$$\langle \varphi_i \varphi_j \dots \varphi_k \varphi_\ell \rangle = \sum_{\text{Wick contractions}} A_{ab}^{-1} \dots A_{cd}^{-1}$$
 (7.72)

For quadratic action functionals, we can therefore calculate any expectation value that we want. Fields with a quadratic action functional are also called "free fields" or non-interacting fields. It's the terms of higher power in the field (typically fourth power) that give interactions, as we will see.

7.6 Massive scalar bosons

7.6.1 Lagrangian density

To finish this chapter, let's outline how to generalize our results from *real* to *complex* scalar fields. As you remember from our discussion of gauge invariance, it is interesting to combine two real scalar (Klein-Gordon) fields φ_R, φ_I into a single complex field $\phi = (\varphi_R + i\varphi_I)/\sqrt{2}$ which has U(1) symmetry. Let's add a source term to the Lagrangian (6.6) that we derived earlier:

$$\mathcal{L}(\phi,\partial_{\mu}\phi) = \partial^{\mu}\phi^{*}\partial_{\mu}\phi - m^{2}\phi^{*}\phi + J^{*}\phi + J\phi^{*}.$$
(7.73)

You see that we have taken care to keep the U(1) symmetry – as long as the source term transforms in the same way as the scalar field, everything is going to be fine. In fact, using $J = (J_R + iJ_I)/\sqrt{2}$ and $\phi = (\varphi_R + i\varphi_I)/\sqrt{2}$, you see that

$$J^{*}\phi + J\phi^{*} = \frac{1}{2} \left[(J_{R} - iJ_{I}) \left(\varphi_{R} + i\varphi_{I}\right) + (J_{R} + iJ_{I}) \left(\varphi_{R} - i\varphi_{I}\right) \right]$$

$$= J_{R}\varphi_{R} + J_{I}\varphi_{I}, \qquad (7.74)$$

so all we really did is add a source term to both the φ_R Klein-Gordon Lagrangian and the φ_I Klein-Gordon Lagrangian. Indeed, if we substitute ϕ, ϕ^*, J and J^* into Lagrangian (7.73) we get

$$\mathcal{L}(\phi,\partial_{\mu}\phi) \rightarrow \frac{1}{2}\partial^{\mu}\varphi_{R}\partial_{\mu}\varphi_{R} - \frac{m^{2}}{2}\varphi_{R}^{2} + J_{R}\varphi_{R} + \frac{1}{2}\partial^{\mu}\varphi_{I}\partial_{\mu}\varphi_{I} - \frac{m^{2}}{2}\varphi_{I}^{2} + J_{I}\varphi_{I}$$
(7.75)

There are *still* two independent variables, as we need to integrate over the complex plane. We could use φ_R, φ_I as integration variables or ϕ, ϕ^* , since the Jacobian corresponding to the change of integration variables equals one:

$$\left| \begin{pmatrix} \partial \phi / \partial \varphi_R & \partial \phi / \partial \varphi_I \\ \partial \phi^* / \partial \varphi_R & \partial \phi^* / \partial \varphi_I \end{pmatrix} \right| = \left| \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ 1/\sqrt{2} & -i/\sqrt{2} \end{pmatrix} \right| = |-i| = 1$$
(7.76)

This also clarifies why we introduce the $1/\sqrt{2}$ factor. We note $\int \mathcal{D}\varphi_R \int \mathcal{D}\varphi_I = \int \mathcal{D}\phi$, keeping in mind that $\int \mathcal{D}\phi$ integrates over two independent variables.

7.6. MASSIVE SCALAR BOSONS

7.6.2 Conserved current

It is important that you do not mix the source terms from (7.73) up with the conserved 4-current which is the Noether current for the U(1) symmetry! Let's figure out what this conserved current is. The U(1) symmetry changes $\phi \to \phi e^{i\alpha}$. So the infinitesimal change in the field is $\phi \to \phi + i\varepsilon\phi = \phi + \varepsilon\delta\phi$ with

$$\delta\phi = \frac{1}{\sqrt{2}} \left(i\varphi_R - \varepsilon\varphi_I \right) \Rightarrow \begin{cases} \delta\varphi_R = -\varphi_I \\ \delta\varphi_I = +\varphi_R \end{cases} .$$
(7.77)

We get

$$J^{\mu} = \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi_{R})} \delta \varphi_{R} + \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi_{I})} \delta \varphi_{I}$$

$$= -\varphi_{I} \partial^{\mu} \varphi_{R} + \varphi_{R} \partial^{\mu} \varphi_{I}. \qquad (7.78)$$

As you see, when multiple field (components) are present, we have to add up all the contributions. Writing this back into complex fields we get

$$J^{\mu} = i \left(\phi \partial^{\mu} \phi^* - \phi^* \partial^{\mu} \phi \right) \tag{7.79}$$

The confusing thing is that this complex current will be the sources for the electromagnetic field! The source terms for the complex field itself, J, is another parameter altogether.

7.6.3 Pair expectation

OK, back to business, let's calculate Z(J) for the complex scalar field. We will now get integrations of the type

$$\int \frac{d\varphi_{R,x}}{\sqrt{2\pi}} \int \frac{d\varphi_{I,x}}{\sqrt{2\pi}} \exp\left\{-\phi_x^* a_x \phi_x + J_x^* \phi_x + J_x \phi_x^*\right\}$$

$$= \int \frac{d\varphi_{R,x}}{\sqrt{2\pi}} \exp\left\{-a_x \varphi_{R,x}^2/2 + J_{R,x} \varphi_{R,x}\right\} \int \frac{d\varphi_{I,x}}{\sqrt{2\pi}} \exp\left\{-a_x \varphi_{I,x}^2/2 + J_{R,x} \varphi_{I,x}\right\}$$

$$= \frac{1}{a_x} \exp\left\{\frac{1}{2}a_x^{-1} \left(J_{R,x}^2 + J_{I,x}^2\right)\right\} = \frac{1}{a_x} \exp\left\{J_x^* a_x^{-1} J_x\right\}$$
(7.80)

OK, here I assume we have already diagonalized the matrix A, but I'm out to find the generalization of our results, and do not want to go through all the details of the diagonalization again. From the above, it is already clear what the general result will be for the complex scalar field:

$$Z(J) = Z(0) \exp\left\{\int dx \int dy \ J_x^* A_{xy}^{-1} J_y\right\}$$
(7.81)

with

$$Z(0) = \frac{1}{\det(A)} \tag{7.82}$$

. Moreover, it is now clear that our result for the pair expectation value still holds:

$$\begin{aligned} \langle \phi_a^* \phi_b \rangle &= \left. \frac{d}{dJ_a} \frac{d}{dJ_b^*} \frac{Z(J)}{Z(0)} \right|_{J=0} \\ &= \left. \frac{d}{dJ_a} \frac{d}{dJ_b^*} \exp\left\{ \int dx \int dy \ J_x^* A_{xy}^{-1} J_y \right\} \right|_{J=0} = A_{ab}^{-1}, \end{aligned}$$
(7.83)

but only if one of the members of the pair is a complex conjugate and the other is not! Indeed, all expectation values $\langle \phi_a^* \phi_b^* \rangle = 0$ and $\langle \phi_a \phi_b \rangle = 0$. The reason is that there are no terms in the expansion of the exponential that have only two J's or only two J's (so they don't vanish when setting all J's to zero). Finally, also in the derivation of the Wick formula, there will be no changes. The Wick decomposition formula (7.72) still holds for complex fields, but we need to pair up starred field with unstarred fields, since $\langle \phi_a^* \phi_b^* \rangle = 0 = \langle \phi_a \phi_b \rangle$.

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Chapter 8

Free quantum fields

8.1 Quadratic action functionals

Let's start from the massive scalar boson, including a source term.

$$\mathcal{L} = \partial^{\mu}\phi^{*}\partial_{\mu}\phi - m^{2}\phi^{*}\phi + J^{*}\phi + J\phi^{*}$$
(8.1)

This is the most general (local) Lagrangian of a scalar real field that obeys Lorentz invariance and that is at most quadratic in the field variables. It is important to note that the mass m has got *nothing* to do with the mass points that we introduced in the model for the string – indeed we obtained just $\frac{1}{2}\partial_{\mu}\varphi\partial^{\mu}\varphi$ for that. So, this is a *different* sort of parameter. The mass term

$$V(\phi) = m^2 \left|\phi\right|^2 \tag{8.2}$$

acts as a potential that wants to bring back all the string segments (both for φ_R and φ_I) to $\varphi_{x,t} = 0$, i.e. to the vacuum state. The action functional can be rewritten as

$$S = \int dx \left\{ \partial^{\mu} \phi^{*} \partial_{\mu} \phi - m^{2} |\phi|^{2} + J^{*} \phi + J \phi^{*} \right\}$$
$$= \int dx \left\{ -\phi^{*} \left(\partial_{\mu} \partial^{\mu} + m^{2} \right) \phi + J^{*} \phi + J \phi^{*} \right\}$$
(8.3)

In the second part, an integration by parts has been performed. The boundary term $\phi^* \partial^{\mu} \phi$ will vanish if we're correct in our assumption that the fields and their associated currents will vanish off sufficiently rapidly when we go to infinity. It's intuitively clear that the mass term helps to localize any disturbance close to its source, but we will need to keep this assumption in mind and check it later. The central quantity that we want to investigate is now

$$Z(J) = \int \mathcal{D}\phi \, \exp\left\{-i \int dx \, \phi^* \left(\partial_\mu \partial^\mu + m^2\right) \phi + i \int dx \, \left(J^* \phi + J \phi^*\right)\right\} \tag{8.4}$$

where the integrals are over spacetime and we set $\hbar = 1$. This is the second fundamental constant that we use to build our set of units, we already set c = 1. We can use identify the linear operator

$$A = i \left(\partial_{\mu} \partial^{\mu} + m^2\right) \tag{8.5}$$

as the continuum case of our matrix A_{xy} :

$$Z(J) = \int \mathcal{D}\phi \exp\left\{-\int dx \ \phi^{*}(x) \left(A[\phi]\right)(x) + \int dx \ \left[iJ^{*}(x)\phi(x) + iJ(x)\phi^{*}(x)\right]\right\}$$
(8.6)

With respect to our previous notations we have an extra factor i in A, and we also have iJ in stead of J. So we have to be careful, now we will no longer be dealing with Gaussian integrals but with oscillating integrals of the type

$$\int_{-\infty}^{\infty} e^{-iau^2} du \tag{8.7}$$

in stead. Bad luck: it doesn't converge. The coefficient of $|\phi|^2$ in the Gaussian integral should not be purely imaginary. In fact, to use our results from Gaussian integration, the coefficient of $|\phi|^2$ needs to have a nonnegative real part, which, however, can be infinitesimally small. This is taken into account by requiring a small imaginary contribution to the mass:

$$m^2 \to m^2 - i\varepsilon$$
 (8.8)

with which we get what we need: the ε term lets the infinite number of integrations in

$$\int \mathcal{D}\phi \, \exp\left\{-i \int dx \, \phi^*(x) \left(\partial_\mu \partial^\mu + m^2\right) \phi(x) - \varepsilon \int dx \, \left|\phi(x)\right|^2\right\}$$
(8.9)

converge. As is customary, such infinitesimals are treated with a generic notation ε , such that any real positive number multiplied with ε is still written as ε : it remains a number that we can choose as small as we want. Let's put this ε -rabbit in the hat, so we can conjure up its magic when needed. With this ε in the back of our mind, we can use our previous result obtained with Gaussian integrations, expression (7.81):

$$Z(J) = Z(0) \exp\left\{-\int dx \int dy \ J^*(x) \ A_{xy}^{-1} \ J(y)\right\}$$
(8.10)

The minus sign comes from replacing $J \to iJ$ twice. Now the difficulty of course lies in figuring out A_{xy}^{-1} ...

8.2 Green's functions

8.2.1 In real space...

To find the operator A^{-1} we rely on the definition of the inverse: it must satisfy $A^{-1}A = AA^{-1} = 1$. In the discretized version this is $A_{jk}A_{k\ell}^{-1} = \delta_{j\ell}$. In the continuum limit this becomes a linear operator

$$A = i \left(\partial_{\mu} \partial^{\mu} + m^2\right) \tag{8.11}$$

And we will introduce a new notation convention for the inverse operator:

$$A_{xy}^{-1} = iD(x-y) \tag{8.12}$$

We know that D(x, y) must actually be a function of x - y, since we have a homogenous problem in space. With this notation our result (8.10) becomes

$$Z(J) = Z(0) \exp\left\{-i \int dx \int dy \ J^*(x) D(x-y) J(y)\right\}.$$
 (8.13)

By convention we defined D(x-y) with a factor *i* in order to cancel the *i* in A, so that the continuum limit of $A_{jk}A_{k\ell}^{-1} = \delta_{j\ell}$ becomes

$$-\left(\partial_{\mu}\partial^{\mu} + m^{2}\right)D(x-y) = \delta(x-y), \qquad (8.14)$$

The above expression in fact tells us that we are looking for the Green's function of the Klein-Gordon equation. More precisely, we need to determine the Green's function corresponding to the piece between the field operators in the action's quadratic term $\phi^* \left[-(\partial_\mu \partial^\mu + m^2) \right] \phi$.

It is important to note that D(x-y) is not only the Green's function of the field equation, it is also the *pair expectation value* $\langle \phi(x)\phi^*(y)\rangle$. Indeed, we can derive (8.6) with respect to iJ twice to bring down the two ϕ 's:

$$\langle \phi(x)\phi^*(y)\rangle = \frac{\delta}{\delta [iJ(y)]} \frac{\delta}{\delta [iJ^*(x)]} \frac{Z(J)}{Z(0)} \Big|_J$$

$$= -\frac{\delta}{\delta J(y)} \frac{\delta}{\delta J^*(x)} \frac{Z(J)}{Z(0)} \Big|_J$$
(8.15)

Substitution of (8.13) into this yields

$$D(x-y) = -i \langle \phi(x)\phi^*(y) \rangle$$
(8.16)

We will often write the result (8.13) for Z(J) as

$$Z(J) = e^{iW(J)} \tag{8.17}$$

Here W(J) is the phase acquired by Z due to the presence of the source field J(x),

$$W(J) = -\int dx \int dy J^*(x) D(x-y) J(y).$$
 (8.18)

If the system has acquired an energy E (due to the presence of the sources), we know that the time evolution (over a time T) of the amplitude to be in this state will be proportional to e^{-iET} (with $\hbar = 1$). Hence we can relate this phase shift W(J) to the energy shift due to the sources: E(J) = -W(J)/T.

8.2.2 ...and in reciprocal space

You can look up the Green's function for a large number of (partial) differential equations in books. Here we rely on the fact that whereas A is not diagonal in position representation, it is diagonal in reciprocal space! We choose the following sign convention for the Fourier transform of the fields:

$$\phi(k) = \int dx \ e^{-ikx}\phi(x) \tag{8.19}$$

$$\Rightarrow \quad \phi(x) = \int \frac{dk}{(2\pi)^4} e^{+ikx} \phi(k). \tag{8.20}$$

whence we get the integral representations of the delta function:

$$\delta(x-y) = \int \frac{dk}{(2\pi)^4} e^{ik(x-y)}$$
(8.21)

It is instructive to write this out with three-vectors again,

$$x = \{x^{0}, x^{1}, x^{2}, x^{3}\} = \{x^{0}, \vec{x}\} = \{t, \vec{x}\}$$

$$k = \{k_{0}, k_{1}, k_{2}, k_{3}\} = \{k_{0}, -\vec{k}\} = \{\omega, -\vec{k}\}$$

$$\Rightarrow e^{-ikx} = e^{-ik_{\mu}x^{\mu}} = e^{-i\omega t}e^{+i\vec{k}\cdot\vec{x}}$$
(8.22)

The spatial 3-vector \vec{k} gets a minus sign since k is assumed covariant¹ in the product kx. We also Fourier transform the source term

$$J(k) = \int dx \ e^{-ikx} J(x) \Leftrightarrow J(x) = \int \frac{dk}{(2\pi)^4} e^{+ikx} J(k)$$
(8.23)

and the propagator:

$$D(k) = \int dx \ e^{-ik(x-y)} D(x-y) \Leftrightarrow D(x-y) = \int \frac{dk}{(2\pi)^4} \ e^{+ik(x-y)} D(k) \ (8.24)$$

Let's use (8.21) and (8.24) in (8.14):

$$-\left(\partial_{\mu}\partial^{\mu}+m^{2}\right)\left(\int\frac{dk}{(2\pi)^{4}}\ e^{+ik(x-y)}D(k)\right) = \left(\int\frac{dk}{(2\pi)^{4}}e^{ik(x-y)}\right)$$
(8.25)

¹Multiplying by k in reciprocal space is like deriving with respect to x, and that is the prototype covariant vector.

8.3. PROPAGATING PARTICLES

The derivative (with respect to x^{μ} bring down factors ik_{μ}):

$$\Leftrightarrow \int \frac{dk}{(2\pi)^4} e^{+ik(x-y)} \left[\left(-k^{\mu}k_{\mu} + m^2 \right) D(k) - 1 \right] = 0$$
 (8.26)

This is satisfied all x - y if and only if all Fourier components are zero:

$$\Leftrightarrow D(k) = \frac{1}{k^{\mu}k_{\mu} - m^2}$$
(8.27)

The fact that we now get a simple result, $D = 1/(k^2 - m^2)$ was actually the motivation for our sign convention. The inverse Fourier transform then gives us

$$D(x-y) = \int \frac{dk}{(2\pi)^4} \frac{e^{ik(x-y)}}{k^2 - m^2 + i\varepsilon}$$
(8.28)

where we took the rabbit out of the hat since we have the dangerous possibility of poles here. Indeed, simply plugging in $D(k) = -1/(k^2 - m^2)$ leads to a divergent integral. Indeed, there are poles at

$$k^{2} - m^{2} = 0 \Leftrightarrow \omega^{2} - \vec{k}^{2} - m^{2} = 0 \Leftrightarrow \omega = \pm \omega_{k}$$

with $\omega_{k} = \sqrt{\vec{k}^{2} + m^{2}}$ (8.29)

Now we can plug in our result for D(x - y) into the $Z(J) = Z(0)e^{iW(J)}$ and find

$$W(J) = -\int dx \int dy \ J^*(x) \int \frac{dk}{(2\pi)^4} \frac{e^{ik(x-y)}}{k^2 - m^2 + i\varepsilon} J(y)$$
(8.30)
$$= -\int \frac{dk}{(2\pi)^4} \left(\int dx J^*(x) e^{ikx} \right) \frac{1}{k^2 - m^2 + i\varepsilon} \left(\int dy J(y) e^{-iky} \right)$$

from which:

$$W(J) = -\int \frac{dk}{(2\pi)^4} J^*(k) \frac{1}{k^2 - m^2 + i\varepsilon} J(k)$$
(8.31)

8.3 Propagating particles

[This part is described magnificently in the book of Zee, and I just use his text with some small modifications]

The source term describes how our springy string is being disturbed. We can choose any function we like, corresponding to our freedom to push and pull the string wherever and whenever we like. Typically, J(x) can be localized in space and time. By tapping the string we can get wave packets going off along the string – or we can stop a wavepacket. Hence J(x) corresponds to sources or sinks of such wave packets.



Figure 8.1: An initial kick J_1 is the source of a propagating disturbance – the particle associated with the field. It can be absorbed by a proper counterkick from the sink at J_2 .

Up till now we talked about fields, not particles. So what do we mean with the "field for phonons" or the "field for electrons" – where is the phonon or the electron in our story? Here's a first very important thing to realize: **the particle associated with the field has got nothing to do with the mass points we used in our discretized springy string model**. That's why the "mass" in the mass term was also unrelated to the points in our springy string model. So what are the particles associated with the field? They are precisely the wave packets that we generate in sinks and absorb in the sources!

More precisely, they are the **excitation quanta of the field**. Take our violin string for example. You can excite a wave on it, and classically the wave can take any amplitude. That's not true quantum mechanically, there the amplitude is quantized. The smallest amplitude corresponds to 1 quantum of excitation. We could call the particle associated with our model the "stringon", and it would be a boson (because scalar real fields commute).

Finally, D(x - y) tells us how the influence of a source at x spreads out in spacetime over a distance x - y. In other words, D(x - y) tells us how the particles propagate from one spacetime point x to another spacetime point y. Therefore D is also called the **propagator**.

Let's have a look again at (8.31), and like in figure 8.1, take $J(x) = J_1(x) + J_2(x)$ where J_1 and J_2 are concentrated in two local regions 1 and 2 in spacetime. Hence, W(J) will have four terms corresponding to the combinations $J_1^*J_1$, $J_1^*J_2$, $J_2^*J_1$ and $J_2^*J_2$. Let's focus on the heterogeneous terms, such as

$$W(J) = -\int \frac{dk}{(2\pi)^4} J_1^*(k) \frac{1}{k^2 - m^2 + i\varepsilon} J_2(k)$$
(8.32)



Figure 8.2: The function D(k) is plotted for m = 1 and $\varepsilon = 0.2$. It is peaked along $k^2 = m^2$, i.e. $\omega^2 = \vec{k}^2 + m^2$, but it is also smeared out. In red we have the classical dispersion relation $\hbar\omega = (\hbar \vec{k})^2/(2m) + mc^2$ (for our choice $\hbar = m = c = 1$), matching the relativistic case only for low energies. Blue to red shades correspond to a [-5, 5] range.

This influence on Z_J will be large only if $J_1(x)$ and $J_2(x)$ overlap significantly in their Fourier transforms and if in the region of overlap in momentum space $1/(k^2 - m^2 + i\varepsilon)$ becomes very large. We interpret the physics contained in our simple field theory model precisely as illustrated in figure 8.1: in region 1 in spacetime there exists a source that sends out a "disturbance in the field" which is later absorbed by a sink in region 2 in spacetime.

Experimentalists choose to call this disturbance in the field a particle of mass m. There is a resonance-like spike at $k^2 = m^2$, that is, if the energymomentum relation of a particle of mass m is satisfied. This is clearly visible in figure 8.2: the amplitude is concentrated along the curve ω_k , expression (8.29). Putting in the necessary \hbar 's and c's this condition is nothing but $p_{\mu}p^{\mu} = m^2 \Leftrightarrow$ $E^2 - (pc)^2 = m^2 c^4 \Leftrightarrow \omega = \pm \omega_k$, the special relativity energy formula. Whereas classically only one value of k contributes², here we must integrate over all k's. Indeed, classically we only have the delta-function like red curve, and zero outside. The quantum field propagator is smeared out as it has nonzero value also for $k^2 \neq m^2$.

The propagator D(k) is peaked in reciprocal space, so it will be wavy in real spacetime. We show (the real part of) D(x) in the left panel of figure 8.3. The light cone is clearly visible: inside the cone the oscillations occur, indicating that

²When $k^2 = m^2$, k is said to be "on mass shell".



Figure 8.3: The real part of our propagator D(x-y) from field theory is shown in the left panel, for disturbances starting in y = 0. The (real part of the) quantum mechanical amplitude to get from the origin to a spacetime point $\{x, t\}$ is shown in the right panel. These are basically the fourier transforms of figure 8.2. Red is large and positive, blue is large and negative, and the pale color is zero. The relativistic propagator goes to zero over a distance $\propto 1/m$ outside of the light cone.

particles can propagate. Outside the light cone, the propagator drops quickly to zero. As you can see looking closely at the origin, there is a bit of quantum mechanical amplitude leaking out of the light cone. However, it cannot get far: it leaks out only over a distance equal to the Compton wavelength \hbar/mc (for these figures, we set $m = c = \hbar = 1$), which is inversely proportional to its mass. In the right panel we show the quantum mechanical amplitude for a single free particle to propagate from the origin to any spacetime point $\{x, t\}$. In the regions outside the light cone (black lines), things obviously go wrong! We find that the quantum waves propagate all over the forbidden region, but in fact we already knew to expect this since regular quantum mechanics is not covariant, and it is precisely the marriage between special relativity and quantum mechanics that led us to quantum field theory. Note that if you stick to the x = 0 world line (very slow particles), the oscillations between blue and red bands are precisely the same, just as they should be in the non-relativistic limit!

8.4 Force mediated by particle exchange

Particles can be the carrier of forces, especially bosonic particles. Rather than having the lads from figure 8.1 jumping up or down, we could let them just sit

8.4. FROM PARTICLE TO FORCE

around like lazy burns. Then $J_1(x) = \delta^{(3)}(\vec{x} - \vec{x}_1)$ and $J_2(x) = \delta^{(3)}(\vec{x} - \vec{x}_2)$ are independent of time. Now $J(x) = J_1(x) + J_2(x)$ is the sum of sources that are time-independent infinitely sharp spikes located at \vec{x}_1 and \vec{x}_2 . What do the quantum fluctuations in the field $\phi_{x,t}$, i.e. the vibrations in our line-mattress, do to the two lumps sitting on the mattress ? If you expect an attraction between the two lumps then you are quite right.

As before W(J) contains four terms. We neglect the $J_1^*J_1$ contribution – this represents a self-induced potential, the dimple in the mattress generated by the lump sitting on it. It is present regardless or not of the presence of the second lump. To study the interaction between the two massive lumps we first find

$$J_{1}^{*}(k) = \int dx \ J_{1}(x)e^{ikx}$$

= $\int dt \int d^{3}\vec{x} \ \delta^{(3)}(\vec{x} - \vec{x}_{1}) \exp\left\{ik^{0}t - i\vec{k} \cdot \vec{x}\right\}$
= $e^{-i\vec{k}\cdot\vec{x}_{1}} \int dt \ e^{ik_{0}t}$ (8.33)

and

$$J_2(k) = e^{+i\vec{k}\cdot\vec{x}_2} \int dt' \ e^{-ik_0t'}$$

This can be substuted in (8.32) to obtain

$$W(J) = -\left(\int dt' \ e^{-ik_0t'}\right) \left(\int dt \ e^{ik_0t}\right) \int \frac{dk}{(2\pi)^4} \ e^{-i\vec{k}\cdot\vec{x}_1} \frac{1}{k^2 - m^2 + i\varepsilon} e^{+i\vec{k}\cdot\vec{x}_2}$$

We can use one of the time integrals, $\int dt' e^{-ik_0t} = (2\pi) \,\delta(k^0 = 0)$ to fix k^0 . This means that the main contribution will certainly not be on-shell, since $(k^0)^2 - \vec{k}^2 \rightarrow -\vec{k}^2$ can never become equal to the positive quantity m^2 . Now we can use the delta function to remove the k^0 integral (and fill in $k^0 = 0$ everywhere in the integrand) and obtain

$$W(J) = -\int dt \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{e^{-i\vec{k}\cdot(\vec{x}_1-\vec{x}_2)}}{-\vec{k}^2 - m^2 + i\varepsilon}$$
(8.34)

We have already mentioned that the quantum mechanical amplitude Z(J) can also be expressed by saying that we start with vacuum $|\emptyset\rangle$, then evolve this in time $e^{-i\hat{H}T} |\emptyset\rangle$, and finally project it back on vacuum $\langle\emptyset|$, so

$$\frac{Z_J}{Z_0} = \langle \emptyset | e^{-i\hat{H}T} | \emptyset \rangle = e^{-iET}$$
(8.35)

where E is the energy difference between having two lumps $J \neq 0$ and no lumps J = 0. The presence of the fluctuating bosonic field has lead to a nonzero change in energy, that we can calculate from E = -W/T where $T = \int_0^T dt$ takes care

of the weird integral over time. The energy change due to the presence of the second lump is then

$$E = -\int \frac{d^3\vec{k}}{(2\pi)^3} \frac{e^{-i\vec{k}\cdot(\vec{x}_1 - \vec{x}_2)}}{\vec{k}^2 + m^2 - i\varepsilon},$$
(8.36)

We can drop the $i\varepsilon$ term, now it is no longer needed to keep the integrand from diverging so we cat let $\varepsilon \to 0$. The presence of the second lump has lowered the energy: the two sources attract each other due to the presence of the φ field! Indeed, even without doing the integral, we see that as $\vec{r} = \vec{x}_1 - \vec{x}_2$ gets larger the oscillatory factor cuts the integral.

Let's perform the integrations and find E. In spherical coordinates $\{\hat{k}, \theta, \phi\}$ for \vec{k} we obtain

$$E = -\frac{1}{(2\pi)^2} \int_0^\infty d\tilde{k} \ \tilde{k}^2 \int_{-1}^1 dx \frac{e^{-i\tilde{k}rx}}{\tilde{k}^2 + m^2}$$

$$= -\frac{1}{(2\pi)^2} \int_0^\infty d\tilde{k} \ \tilde{k}^2 \frac{e^{-i\tilde{k}r} - e^{+i\tilde{k}r}}{-i\tilde{k}r} \frac{1}{\tilde{k}^2 + m^2}$$

$$= \frac{1}{(2\pi)^2 ir} \left(\int_0^\infty d\tilde{k} \ \frac{\tilde{k}e^{-i\tilde{k}r}}{\tilde{k}^2 + m^2} - \int_0^\infty d\tilde{k} \ \frac{\tilde{k}e^{+i\tilde{k}r}}{\tilde{k}^2 + m^2} \right)$$

In the second term, we set $\tilde{k} \to -\tilde{k}$, to obtain

$$E = \frac{1}{(2\pi)^2 ir} \left(\int_0^\infty d\tilde{k} \frac{\tilde{k}e^{-i\tilde{k}r}}{\tilde{k}^2 + m^2} + \int_{-\infty}^0 d\tilde{k} \frac{\tilde{k}e^{-i\tilde{k}r}}{\tilde{k}^2 + m^2} \right)$$
$$= \frac{1}{(2\pi)^2 ir} \int_{-\infty}^\infty d\tilde{k} \frac{\tilde{k}e^{-i\tilde{k}r}}{\left(\tilde{k} + im\right)\left(\tilde{k} - im\right)}$$

The denominator has been factorized to show the location of the poles. We solve this integral by contour integration along a large halve circle. The factor $e^{-i\tilde{k}r}$ forces us to close the contour along the lower half complex plane since r > 0. The contour then only contains the pole at $\tilde{k} = -im$, and moreover is traversed in clockwise sense, introducing a minus sign. We find

$$E = -\frac{1}{(2\pi)^2 ir} 2\pi i \operatorname{Res}_{\tilde{k}=im} \left(\frac{\tilde{k}e^{-i\tilde{k}r}}{\left(\tilde{k}+im\right)\left(\tilde{k}-im\right)} \right)$$

$$\Rightarrow E = -\frac{1}{4\pi r} e^{-mr}$$
(8.37)

The result is as we expected: the energy drops off exponentially over a distance scale $\propto 1/m$. This distance scale is of course again the Compton wavelength –

the typical length scale where relativistic effects become important in quantum theory, and vice versa. The resulting force F = -dE/dr is attractive (and also limited in range). The fluctuating scalar real field mediates an attractive interaction between particles that couple to it. Yukawa proposed that the attraction between nucleons in the atomic nucleus is due to precisely such a coupling. Now we know that this is true, and that the particle associated with the field is the π -meson or the pion.

Summarizing what we have thus far:

(1) The Green's function of the field equation = the pair expectation value = the amplitude of propagation of the particle associated with the field

(2) Integrating out a free bosonic field can be done exactly and leads to an interaction between sources coupled to that field, this interaction can be interpreted as the sources exchanging a boson that propagates from one to the other.

Of course, the sort of interaction you get depends on the type of beast that populates your spacetime. There's many more possibilities than scalar real fields. In the next section we explore one interesting alternative: the complex vector field.

8.5 Massive vector bosons

8.5.1 Their (quadratic) action,

Back in our section on gauge theories, we found that imposing U(1) invariance led us to introduce a (real) vector field A^{μ} such that the Lagrangian is:

$$\mathcal{L} = (\partial^{\mu} - iA^{\mu})\phi^{\dagger}(\partial_{\mu} - iA_{\mu})\phi - m^{2}\phi^{\dagger}\phi - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}$$
(8.38)

This describes a particle (associated with the field ϕ) interacting with the electromagnetic field. The interaction terms are the cross-terms

$$-i\left(\phi^{\dagger}\partial_{\mu}\phi + \phi\partial_{\mu}\phi^{\dagger}\right)A^{\mu} = J_{\mu}A^{\mu}$$
(8.39)

since the prefactor in A^{μ} corresponds to the 4-current in the field ϕ . This is the conserved quantity $\partial^{\mu} J_{\mu} = 0$ linked to translation invariance, better known in some circles as electric charge and electric current! So, if we focus on the electromagnetism part of the Lagrangian, we find that it is described by

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + J_{\mu} A^{\mu}$$
 (8.40)

Indeed, this represents the Lagrangian of electromagnetism – its classical field equations are the Maxwell equations! So, the electromagnetic force is carried by the quanta of excitation of the complex vector field A^{μ} : the photons. We won't study this yet, we're first going to give photons a mass (taking the mass $\rightarrow 0$ limit is a bit tricky, just try it in the propagator for the scalar boson...). It's no longer a photon there, but a massive vector boson. The Lagrangian becomes

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{M^2}{2}A_{\mu}A^{\mu} + A^{\mu}J_{\mu}$$
(8.41)

After some partial integrations (and vanishing boundary terms) we can reshuffle the terms in the action functional to read

$$S = \int dx \left\{ \frac{1}{2} A_{\mu} \left[\left(\Box + M^2 \right) g^{\mu\nu} - \partial^{\mu} \partial^{\nu} \right] A_{\nu} + A_{\mu} J^{\mu} \right\}$$
(8.42)

This equivalence is one of the questions in your problem sets so I won't prove it here³. However, note that for the scalar field we had $-\phi^* (\Box + M^2) \phi$: in the action functional: an additional minus sign.

8.5.2 their Green's function,

What will be its Green's function ? It has to be the operator $D_{\mu\nu}(x-y)$ that inverts the operator $(\Box + M^2) g^{\mu\nu} - \partial^{\mu} \partial^{\nu}$. This means it has to satisfy the equation

$$\left[\left(\Box + M^2\right)g^{\mu\nu} - \partial^{\mu}\partial^{\nu}\right]D_{\nu\lambda}(x-y) = \delta^{\mu}_{\lambda}\delta^{(4)}(x-y)$$
(8.43)

Note that now the Green's function is a rank-2 tensor. Massive vector bosons can move from x to y but also scramble up their components while doing so, $D_{\mu\nu}$ tells you how much of the ν component has been mixed into the amplitude of the μ component after its travel between x and y.

We find the Green's function again by going to reciprocal space, where it has to satisfy

$$\left[-\left(k^{2}-M^{2}\right)g^{\mu\nu}+k^{\mu}k^{\nu}\right]D_{\nu\lambda}(k)=\delta_{.\lambda}^{\mu.}$$
(8.44)

The solution is

$$D_{\nu\lambda}(k) = \frac{-g_{\nu\lambda} + k_{\nu}k_{\lambda}/M^2}{k^2 - M^2}$$
(8.45)

We can again add a $+i\varepsilon$ in the denominator to prevent it from blowing up the whole expression. Now we have $iD_{\nu\lambda}(x-y) = \langle A_{\nu}(x)A_{\lambda}(y) \rangle$.

³Note that if we choose the Lorentz gauge, $\partial^{\nu}A_{\nu} = 0$, then the field equations corresponding to this action functional are $(\Box + m^2) A_{\mu} = 0$, so each component of the 4-vector A_{μ} obeys the Klein-Gordon equation!

8.5.3 and the force they mediate

We can then plug our result back into

$$W(J) = -\frac{1}{2} \int dx \int dy \ J^{\mu}(x) D_{\mu\nu}(x-y) J^{\nu}(y)$$
 (8.46)

$$= -\frac{1}{2} \int \frac{d^3k}{(2\pi)^3} (J^{\mu}(k))^* D_{\mu\nu}(k) J^{\nu}(k), \qquad (8.47)$$

where now the source terms are 4-currents. Ah yes, the charge and current density in this 4-vector are the sources of electric and magnetic fields! Another good reason to call these the source terms. We get

$$W(J) = -\frac{1}{2} \int \frac{d^3 \vec{k}}{(2\pi)^3} \left(J^{\mu}(k) \right)^* \frac{-g_{\mu\nu} + k_{\mu}k_{\nu}/M^2}{k^2 - M^2} J^{\nu}(k).$$
(8.48)

Wonderful news: current conservation $\partial_{\mu}J^{\mu} = 0$ is expressed in reciprocal space as $k_{\mu}J^{\mu} = 0$. Hence, we can throw away the $k_{\mu}k_{\nu}$ part of the propagator, and get

$$W(J) = +\frac{1}{2} \int \frac{d^3 \vec{k}}{(2\pi)^3} \frac{1}{k^2 - M^2} J_{\mu}(k) \left(J^{\mu}(k)^*\right)$$
(8.49)

Take notice of the sign change! Now we put the two lumps in the field. We only place charges, no currents, so there is only a J^0 component. We get $J^0(x) = \rho_a \delta^{(3)}(\vec{x} - \vec{x}_a) + \rho_b \delta^{(3)}(\vec{x} - \vec{x}_b)$. The derivation that we had for the scalar field can simply be copied here, we get

$$E(r) = +\frac{\rho_a \rho_b}{4\pi r} e^{-Mr} \tag{8.50}$$

The factor 1/2, in the original A, is canceled here when we combine $J_1^*J_2$ and $J_2^*J_1$ terms. As we let the mass go to zero, our vector boson becomes more and more like a photon, and we obtain Coulomb's law, $F \approx \rho_a \rho_b/(4\pi r^2)$. The sign change results in repulsion between like charges. There it is: electrostatics derived from local gauge invariance, in little over two pages, bypassing Maxwell.

CHAPTER 8. FREE QUANTUM FIELDS

Chapter 9

Interacting fields

9.1 Anharmonicity and ϕ^4 -theory

We could perform the integrations from the previous chapter analytically, because they were all (multivariate) Gaussian integrals. That is because we made the approximation that the springy string is, well... springy. The mass points in the string are connected with harmonic springs, and as a result the vibrational modes can be superposed. The "phonons" or lattice oscillations pass right through each other and cannot scatter off each other. There are no interactions between the elementary excitations of the field, i.e. between the particles corresponding to the field. Of course, charges coupled to the electromagnetic field interact by exchanging photons, but the photons themselves do not interact.

However, this is not the case in general ! Including these interactions means adding anharmonicity to the springs, and this results in a field Lagrangian such as

$$\mathcal{L} = \partial_{\mu} \phi^* \partial^{\mu} \phi - m^2 \left| \phi \right|^2 - g \left| \phi \right|^4.$$
(9.1)

We added for simplicity just a φ^4 term¹. For simplicity, we take g to be constant in spacetime, i.e. independent of x. This implies that the interactions between the field quanta are local: we have a "contact" interaction potential $V(x-y) = g\delta(x-y)$. This type of interactions is suitable to describe ultracold atomic gases (of bosonic isotopes such as ⁸⁷Rb, ²³Na, ⁷Li).

The main goal of this chapter will be to figure out what happens to Z, to the propagator $\langle \phi_x^* \phi_y \rangle$, and to Wick decompositions for $\langle \phi_a^* \phi_b^* ... \phi_c \phi_d \rangle$ as we switch on g to include interactions.

In order to study Z(g) and the expectation values we found it useful to

¹This is an important example, because if we have two fields φ_R, φ_I that each obey this Lagrangian, and we add interactions between the fields, $2(g/4!) \varphi_R^2 \varphi_I^2$, it is easy to combine them into a single U(1) invariant Lagrangian for $\phi = \varphi_R + i\varphi_I$. Then we just get $(g/4!) |\phi|^4$. So, we get an interacting complex field.

include a source term. So, we're going to investigate

$$Z(J,g) = \int \mathcal{D}\phi \exp\left\{i\int dx \left[-\phi^* \left(\Box + m^2\right)\phi - g \left|\phi\right|^4 + J^*\phi + J\phi^*\right]\right\}$$
(9.2)

Note that the interaction term $g |\phi|^4 = g (\phi^*)^2 \phi^2$ preserves U(1) symmetry, as it is invariant under $\phi \to \phi e^{i\alpha}$.

9.2 Perturbation expansion for Z

9.2.1 Central formula

There's no analytical result for the multi-dimensional integral (??), bummer. Here the great usefulness of the path integral picture stands out: we do not have operators for the fields, just functions. So, we can factorize the exponential! If the fields are operators we can't since $e^{\hat{A}+\hat{B}} \neq e^{\hat{A}}e^{\hat{B}}$ unless \hat{A} and \hat{B} commute. So,

$$Z(J,g) = \int \mathcal{D}\phi \exp\left\{-ig\int |\phi|^4 dx\right\} \exp\left\{i\int \left[-\phi^*\left(\Box + m^2\right)\phi + J^*\phi + J\phi^*\right] dx\right\}$$
(9.3)

Now the trick is to expand the exponential with the interactions:

$$\exp\left\{-i\int dx \ g \left|\phi\right|^{4}\right\} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(ig\right)^{n} \left(\int dx \ \left|\phi_{x}\right|^{4}\right)^{n}$$
(9.4)

Then we obtain Z(J,g) as a perturbation series in successive powers of g:

$$Z(J,g) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-ig\right)^n Z_{(n)}(J)$$
(9.5)

with

$$Z_{(n)}(J) = \int \mathcal{D}\phi \left(\int dx \ |\phi_x|^4 \right)^n \exp\left\{ i \int \left[-\phi^* \left(\Box + m^2 \right) \phi + J^* \phi + J \phi^* \right] dx \right\}$$
(9.6)

The unperturbed n = 0 term is something we already have explored: it is Z(J) for the non-interacting field

$$Z_{(0)}(J) = Z(J,0) = Z(0,0) \exp\left\{-i \int dx \int dy \ J^*(x) D(x-y) J(y)\right\}$$
(9.7)

with

$$D(x-y) = \int \frac{dk}{(2\pi)^4} \frac{e^{ik(x-y)}}{k^2 - m^2 + i\varepsilon}$$
(9.8)

9.2. PERTURBATION EXPANSION FOR Z

How about the n = 1 term? This is

$$Z_{(1)}(J) = \int dx \int \mathcal{D}\phi \ (\phi_x^*)^2 (\phi_x)^2 \times \exp\left\{i \int \left[-\phi^* \left(\Box + m^2\right)\phi + J^*\phi + J\phi^*\right] dx\right\}$$
(9.9)

We know how to bring two powers of ϕ_x and two powers of ϕ_x^* down from the exponent: derive² with respect to the source field!

$$Z_{(1)}(J) = \int dx \, \frac{\partial^2}{\partial J_x^2} \frac{\partial^2}{\partial (J_x^*)^2} \int \mathcal{D}\phi \, e^{i \int \left[-\phi^* \left(\Box + m^2\right)\phi + J^*\phi + J\phi^*\right] dx}$$
$$= \int dx \, \frac{\partial^2}{\partial J_x^2} \frac{\partial^2}{\partial (J_x^*)^2} Z(J,0)$$

Evidently, we get

$$\frac{Z_{(1)}(J)}{Z(0,0)} = \int dx \, \frac{\partial^2}{\partial J_x^2} \frac{\partial^2}{\partial \left(J_x^*\right)^2} \exp\left\{-i \int dx \int dy \, J^*(x) D(x-y) J(y)\right\} \tag{9.10}$$

I've already divided by Z(0,0) because this constant factor is going to appear in every term in the perturbation. Let's use a tilde on Z to indicate we divide it by Z(0,0), writing

$$\tilde{Z}(J,g) = \frac{Z(J,g)}{Z(0,0)} \text{ and } \tilde{Z}_{(n)}(J) = \frac{Z_{(n)}(J)}{Z(0,0)}.$$
(9.11)

For the expectation values we have to divide by this Z(0,0) normalization factor anyway! It is clear how the procedure will generalize for arbitrary n:

$$Z_{(n)}(J) = \int \mathcal{D}\phi \left(\int dx \left(\phi_x^*\right)^2 \left(\phi_x\right)^2 \right)^n \\ \times \exp\left\{ i \int \left[-\phi^* \left(\Box + m^2\right)\phi + J^*\phi + J\phi^* \right] dx \right\}, \quad (9.12)$$

from which

$$\tilde{Z}_{(n)}(J) = \left(\int dx \ \frac{\partial^2}{\partial J_x^2} \frac{\partial^2}{\partial \left(J_x^*\right)^2}\right)^n \exp\left\{-i \int dx \int dy \ J^*(x) D(x-y) J(y)\right\}$$
(9.13)

Resumming the exponential, we get the central identity of quantum field perturbation theory:

$$\tilde{Z}(J,g) = \exp\left\{-ig\int dx \; \frac{\partial^2}{\partial J_x^2} \frac{\partial^2}{\partial (J_x^*)^2}\right\} \exp\left\{-i\int dx\int dy \; J^*(x)D(x-y)J(y)\right\}$$
(9.14)

Expanding both exponentials allows you to find the term with a given power in g and a given power in J's.

²Here I should write functional derivatives in stead of partial derivatives, but if you are accustomed to switching between the discretized and the continuum version, you get what I mean. Check out appendix A if you don't know what functional derivatives are.

9.2.2 A first order example

How do these types of interactions change the energy of the system? We want to find

$$\tilde{Z}(0,g) = \frac{1}{Z(0,0)} \int \mathcal{D}\phi \exp\left\{i \int dx \left[-\phi^* \left(\Box + m^2\right)\phi - g \left|\phi\right|^4\right]\right\}$$
(9.15)

without the source terms which we introduces as auxiliary fields anyway. From the central idendity we know that we have to take derivatives with respect to J_x and J_x^* , and now we only keep the terms that survive when we set J = 0after deriving. The main thing in perturbation theory is always to connect the correct term from the expansion of

$$\exp\left\{-ig\int dx \;\frac{\partial^2}{\partial J_x^2}\frac{\partial^2}{\partial \left(J_x^*\right)^*}\right\} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-ig\right)^n \left(\int dx \;\frac{\partial^2}{\partial J_x^2}\frac{\partial^2}{\partial \left(J_x^*\right)^*}\right)^n, \quad (9.16)$$

with the correct term from the expansion of

$$\exp\left\{-i\int dx\int dy J_x^* D(x-y)J_y\right\} = \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell}}{\ell!} \left(\int dx\int dy J_x^* iD(x-y)J_y\right)^{\ell},$$
(9.17)

given that at the end we set all J's zero.

Let's look at the first order term in g. This means we want one power in ig, implying that we take the n = 1 term in the first exponential. From the second exponential, we then need a term in expansion with precisely two J_x 's and two J_x^* 's. To get this, we need the second term in the expansion of the second exponent, i.e. $\ell = 2$ and

$$\frac{1}{2!} (-1)^2 \int dy \int dz \ J_y^* i D(y-z) J_z \int du \int dv \ J_u^* i D(u-v) J_v \tag{9.18}$$

The functional derivatives keep only y = z = u = v = x, so that we get

$$\tilde{Z}_{(1)}(J=0) = \left(\frac{-1}{2}\right)(-ig)\int dx \left[iD(x-x)\right]^2$$
(9.19)

and

$$\tilde{Z}(0,g) = 1 + \left(\frac{-1}{2}\right) (-ig) \int dx \left[iD(x-x)\right]^2 + \mathcal{O}(g^2)$$
(9.20)

One of the interpretations of the propagator D(x - y) is that it tells us how a field quantum propagates from y to x, traversing the spacetime distance x - y. In our result here, it is a bit weird to see D(x - x). But still we can interpret it as a fluctuations coming from and going to x. In spacetime we could write this as a little loop from x to x. The first order perturbation result (9.19) can then graphically be represented as

$$iD(x-x)$$
 (9.21)

As we have to sum over all possible possibilities, we need to sum over all x where we can have this double-loop thingy.

Can you figure out the second order terms? You'll see that things quickly become complicated. We need to find some systematics, just like Wick found for the expectation values of long products. For these perturbation expansions, Feynman did find systematics! Before we get to that, we need to look at some answers to other questions we posed in the beginning of this chapter.

9.3 Propagator for the interacting system

Let's turn our attention next to the propagator $iD(x - y) = \langle \phi(x)\phi^*(y) \rangle$, now in the *interacting* system. To distinguish it from the non-interacting system, we'll use a subscript 0, and write

$$iD_0(x-y) = \frac{1}{Z(0,0)} \int \mathcal{D}\phi \ \phi(x)\phi^*(y) \exp\left\{i\int \left[-\phi^*\left(\Box + m^2\right)\phi\right]dx\right\}$$
(9.22)

for the propagator at g = 0. Now we want to find

$$iD(x-y) = \frac{1}{Z(0,g)} \int \mathcal{D}\phi \ \phi(x)\phi^*(y) \exp\left\{i \int \left[-\phi^*\left(\Box + m^2\right)\phi - g\left|\phi\right|^4\right] dx\right\}$$
(9.23)

In comparison to the calculation of Z(0,g) we now have two additional field variables, representing a *source* at y and a *drain* at x. This corresponds to two additional derivatives,

$$iD(x-y) = \frac{1}{\tilde{Z}(0,g)} \left. \frac{\partial}{\partial J_x^*} \frac{\partial}{\partial J_y} \tilde{Z}(J,g) \right|_{J=0}$$
(9.24)

Let's not worry about the denominator Z(0,g) for the moment, and focus on the numerator. We can again use the central formula (9.14),

$$iD(x-y) = \sum_{n=0}^{\infty} \frac{1}{n!} (-ig)^n \left(\int dz \; \frac{\partial^2}{\partial J_z^2} \frac{\partial^2}{\partial (J_z^*)^2} \right)^n \frac{\partial}{\partial J_x^*} \frac{\partial}{\partial J_y} \\ \times \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{\ell!} \left(\int du \int dv J_u^* i D_0(u-v) J_v \right)^\ell$$
(9.25)

and figure out which term of the first expansion (9.16) and of the second expansion (9.17) we need to combine to get the right result. Let's do this up to first order perturbation. So, we're looking for the terms of order g, and we need n = 1. With n = 1, we have no less than six derivatives: three with respect to J's and three with respect to J's. This means we need the $\ell = 3$ term – only this term will have non-zero contributions when we set all J's to zero after

taking the derivative. Hence we get

$$iD_{1}(x-y) = (-ig)\frac{(-1)^{3}}{3!} \int dz \frac{\partial^{2}}{\partial J_{z}^{2}} \frac{\partial^{2}}{\partial (J_{z}^{*})^{2}} \frac{\partial}{\partial J_{x}^{*}} \frac{\partial}{\partial J_{y}} \int du_{1} \int dv_{1}$$
$$\times \int du_{2} \int dv_{2} \int du_{3} \int dv_{3} J_{u_{1}}^{*} iD_{0}(u_{1}-v_{1})J_{v_{1}}$$
$$\times J_{u_{2}}^{*} iD_{0}(u_{2}-v_{2})J_{v_{2}}J_{u_{3}}^{*} iD_{0}(u_{3}-v_{3})J_{v_{3}}$$
(9.26)

Whenever u_1, u_2, u_3 is equal to some permutation of z, z, x and v_1, v_2, v_3 is equal to some permutation of z, z, y, we get a nonvanishing result. Counting out the possibilities, you get

$$iD_{1}(x-y) = (-ig)\frac{(-1)^{3}}{3!}\int dz \{3iD_{0}(x-y)iD_{0}(z-z)iD_{0}(z-z) + 6iD_{0}(x-z)iD_{0}(z-y)iD_{0}(z-z)\}$$
(9.27)

We have two types of terms, namely when x, y are in the same propagator, and when they are in a different one. These two possibilities can be graphed as



and

$$iD(z-z)$$

$$iD(z-y) \quad g \quad iD(x-z)$$

$$(9.28)$$

We contruct these graphs by putting two open squares in the 'external' spacetime points x and y. These are the source (a shaded square) in y and the drain (an open square) in x. For the 'internal' spacetime point z we draw a dot, called an interaction vertex. Note that we have some diagrams with loose pieces (the upper graph): these are called disconnected diagrams. The lowe graph is a connected diagrams. These diagrams tell the story of how the quantum associated with the field can propagate. The upper story is kind of boring: nothing happens to the particle propagating from y to x, and meanwhile somewhere in the vacuum there is a little disturbance, a vacuum fluctuation, but it is not affecting the journey of the particle that we are propagating. The lower cartoon tells another story: on its way from y to x, the particle will feel the interaction with strength g, and interact with a particle located at z (which stays there). The path integral prescription is that we have to sum over all possible stories that we can tell about a particle moving from y to x, and we have to sum all the amplitudes corresponding to these sums. The amplitudes are obtained by using (non-interacting) propagators when the particles are just moving around, and interaction vertices g when they some interaction takes place.

It is no coincidence that the piece which is not connected to the open squares is precisely the piece that we found in $\tilde{Z}(0,g)$ in the previous section. Indeed, $\tilde{Z}(0,g)$ did not have any external spacetime points in which we take expectation values. So $\tilde{Z}(0,g)$ will be exactly the sum of all the loose pieces that we can add to make disconnected diagrams. These loose pieces are called the "vacuum polarization". The left graph corresponds to multipling our $D_0(x-y)$ with such a vacuum polarization diagram. If we continue to higher orders, we'll find all sorts of loose pieces hanging around, and they will again sum up to $\tilde{Z}(0,g)$. By dividing $\tilde{Z}(0,g)$ out, we just remove all these pieces! So, in general:

The effect of dividing by $\tilde{Z}(0,g)$ is precisely to cancel all contributions that correspond to disconnected diagrams. If you simply leave them out, you no longer have to divide over $\tilde{Z}(0,g)$.

OK, let's see if we can get to the second order stories. These are stories with two interaction points, so n = 2. This means we get $\ell = 4n = 8$, so that we have 2 + 4n = 10 derivatives, corresponding to 5 propagators. What diagrams can we make that have 5 propagators and 2 interaction vertices? Remember that we have to connect four lines to each interaction vertex (two incoming, two outgoing, corresponding to the two derivatives with respect to J_z^* and the two derivatives with respect to J_z). We also have to connect one line to the source, and one line to the drain. And we want to discard all the diagrams that have loose pieces. After a bit of puzzling, you'll find



and



and finally



These little cartoons are actually the famous *Feynman diagrams*! They bring out the systematics in our calculations.

9.4 Feynman diagrams

9.4.1 In real spacetime

Rather than doing all the tedious accounting work, introducing source terms and making a zillion derivatives, Feynman proposes the following procedure to figure $D_n(x-y)$:

- 1. Draw all possible connected diagrams that have n internal spacetime points (called *vertices*, located at $z_{i=1,..,n}$) and 2 external points, and 2n + 1 lines connecting these points. Each vertex should link up four lines, and the external points have one line connected to them..
- 2. For each line from spacetime point a to b, write down an unperturbed propagator $iD_0(b-a)$.
- 3. For each vertex (each internal point), multiply by a factor -ig
- 4. Integrate over all internal spacetime points $\prod_{j=1..n} \int dz_j$
- 5. Finally, multiply by some nasty numerical factor (coming from the combinatorics of distributing the derivatives over the propagators). We'll worry about this later.

Let's try it out and find $D^{(1)}(x-y)$. We only have one connected diagram, shown in (9.28), so that's step 1. Step 2 leads us to the product D(x-a)D(a-a)D(a-y). Step 3 lets us multiply by ig and finally we find

$$D_1(x-y) \propto (-ig) \int dz_1 \ i D_0(x-z_1) i D_0(z_1-z_1) i D_0(z_1-y) \tag{9.29}$$

We could now plug in the formula for

$$D_0(b-a) = \int \frac{dk}{(2\pi)^4} \frac{e^{ik(b-a)}}{k^2 - m^2 + i\varepsilon}$$

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You see that this would result in a bunch of k integrations on top of all the integrations over internal points that we have to do.... It becomes much simpler if we stick to reciprocal space to start with!

9.4.2 Momentum conservation

First, we need to prove an important point:

4-momentum is conserved in each vertex

In a vertex always four lines come together:



Here, we've added arrows, in order to distinguish D(x - y) from D(y - x). In general, you are propagating from a source to a sink, and you must keep track of that. Already with complex scalar fields it is important. We get integrations of the type

$$\mathcal{I} = \int da \ i D_0(x_1 - a) i D_0(x_2 - a) i D_0(a - x_3) i D_0(a - x_4) \tag{9.30}$$

If we plug in our results for the propagators, we get

$$\mathcal{I} = \int da \int \frac{dk_1}{(2\pi)^4} \int \frac{dk_2}{(2\pi)^4} \int \frac{dk_2}{(2\pi)^4} \int \frac{dk_2}{(2\pi)^4} \int \frac{dk_4}{(2\pi)^4} \frac{ie^{ik_1(x_1-a)}}{k_1^2 - m^2 + i\varepsilon} \\
\times \frac{ie^{ik_2(x_2-a)}}{k_2^2 - m^2 + i\varepsilon} \frac{ie^{ik_3(a-x_3)}}{k_3^2 - m^2 + i\varepsilon} \frac{ie^{ik_4(a-x_4)}}{k_4^2 - m^2 + i\varepsilon}$$
(9.31)

Collecting all the terms with a gives

$$\int da \, \exp\left\{i(k_1+k_2-k_3-k_4)a\right\} = (2\pi)^4 \,\delta(k_1+k_2-k_3-k_4) \tag{9.32}$$

The sum of all incoming 4-momenta is equal to the sum of all outgoing 4momenta. This trick will help us a lot: doing the integrals over the positions of the internal spacetime points leads to delta functions for the momenta. It seems therefore wise to set up the Feynman rules in reciprocal space

9.4.3 Reciprocal space

The procedure outlined by Feynman to find $D^{(n)}(k)$ is

- 1. Draw all possible connected diagrams that have n vertices and 2 external points (a source and a sink of 4-momentum), and connect these by 2n + 1 lines carrying an arrow. Each vertex should link up to four lines.
- 2. Label each line with a four momentum, making sure that in each vertex the 4-momentum is conserved. The source should have an *outgoing* 4-momentum equal to k, and the sink should have an *incoming* 4-momentum equal to k.
- 3. Translate each line into an unperturbed propagator $iD^{(0)}(k_j) = i/(k^2 m^2 + i\varepsilon)$
- 4. Translate each vertex into a vertex factor (-ig)
- 5. Integrate over all 4-momenta that can be freely chosen (i.e. that are not completely determined by the source and drain)
- 6. Multiply by a tricky combinatorial factor, equal to the number of Wick decompositions that result in the diagram.

So, we're ready for $D^{(1)}(k)$. We only have one connected diagram, shown in (9.28). The propagator going from the source to the vertex must carry the momentum k, and so must the propagator going from the vertex to the sink. In the loop, we can have any momentum we want going around. So we get

$$D^{(1)}(k) \propto (-ig)^2 \left(iD^{(0)}(k) \right)^2 \left[\int \frac{dk_1}{(2\pi)^4} iD^{(0)}(k_1) \right]$$
(9.33)

Try to find the expressions corresponding to the second order diagrams to train yourself using the Feynman rules.

9.4.4 Diagrammatics

We gave rules specifically for our interacting scalar bosons, with contact interactions. How about other types of fields, and other types of interactions? They do not change the basic structure of the Feynman diagrammatic techique!

First of all, we may have more than one type of propagator. If we propagate massive vector bosons, we have to use (8.45) in stead. Electrons propagate differently from photons, and again have a different propagator, corresponding to a different type of line. We usually draw electron propagators with full lines, and photon propagators with wiggly lines. There's a whole zoo of particles, and each has its own type of line. Next, there's all sorts of interactions. Each interaction term has its own vertex, that connects only to specific types of lines. For example, the electromagnetic interaction will have vertex that connects two electrons and one photon line. You're not allowed to use it any other way.

When you analyse a specific problem, figure out what kind of lines and vertices you have as your building blocks – what's in the construction set for Feynman diagrams? Once you're nicely laid out the parts, you can start connecting them up and drawing your Feynman diagrams. Then, step #2 of the procedure stays the same: conserve 4-momentum in each vertex. Steps #3 and #4 come with their specific translations – these have been listed in a dictionary titled "diagrammatics" by Veltman and 't Hooft. Step #5 also stays the same. Finally, step #6 is also specified in the diagrammatics book.

It's not the goal of this specific course to make you learn and remember all the possible propagators and vertices and combinatorial factors – specific courses focus on specific needs. The course in electroweak will tell you what lines to use for neutrino's, W and Z bosons and what sort of vertex factors there are. Gluons and quark lines and their vertices are the topic of QCD. Non-relativistic electrons and phonons also have their lines and vertices, and you can learn about them in the advanced solid state course. In this course the idea is to get the general concept accross. Nevertheless, we will look at a specific application later on: quantum electrodynamics. Then you will learn the rules specific for electrons interacting with photons, and you will calculate the amplitudes for specific processes. So, until then, restrain your urge to do all the integrals.

9.5 Particle scattering

Finally, let's look at higher-order correlations such as

$$\langle \phi(x_1)\phi(x_2)\phi^*(y_1)\phi^*(y_2)\rangle \tag{9.34}$$

From the Wick decomposition rule we know that without interactions, this can be written as a sum over all the ways to pair up fields and conjugate fields. There are just two ways here:

$$\langle \phi(x_1)\phi(x_2)\phi^*(y_1)\phi^*(y_2) \rangle = \langle \phi(x_1)\phi^*(y_1) \rangle \langle \phi(x_2)\phi^*(y_2) \rangle + \langle \phi(x_1)\phi^*(y_2) \rangle \langle \phi(x_2)\phi^*(y_1) \rangle = iD_0(x_1 - y_1)iD_0(x_2 - y_2) + iD_0(x_1 - y_2)iD_0(x_2 - y_1)$$
(9.35)

These two Wick pairings between sources and drains can be graphed as



Notice that now we have two source (shaded squares) and two drains (open squares) and we need to connect them. The Wick decomposition tells you to sum over all possible ways to connect those. For our bosons, we need to add the amplitude that the particles have traded place between source and drain as there is no physical way to distinghuish these two alternatives.

If you go to reciprocal space, you just get $iD_0(k_1)iD_0(k_2)$ for both terms. This tells you that if you start with two non-interacting particles, with momenta k_1 and k_2 , then they will just propagate all the way to the drains with those momenta.

Now, let's add interactions. Up to first order in g, we need to add one vertex, and two propagators as I hope is already clear for you. We could construct a diagram such as



Still we start and end with two particles that did not see each other, and end with in the same state as they started. The only thing we did in this diagram is correct the propagation of one of the particles. That is, we get $iD_0(k_1)iD_1(k_2)$. Adding such diagrams to all orders, we'd get $iD(k_1)iD(k_2)$. However, there is a more interesting thing that we can do with one vertex and four lines:



we can use the vertex to link up the particles. Conservation of momentum in the vertex tells us that the particles must exchange a 4-momentum q during this interaction. This diagram represents the simplest sort of scattering between two particles. They start with k_1, k_2 , then collide (with amplitude ig) and scatter off with momenta $k_1 - q$ and $k_2 + q$. The quantum mechanical amplitude for this process is

$$T(k_1, k_2; q) \propto (-ig) i D_0(k_1) i D_0(k_2) i D_0(k_1 - q) i D_0(k_2 + q)$$
(9.36)

Taking higher order processes into account, we can sum up all diagrams where the particles start with $\{k_1, k_2\}$ and end up with $\{k_1 - q, k_2 + q\}$. This scattering amplitude is called the *T*-matrix. The modulus square of it will give the

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probability of such scattering processes and is a measurable quantity: throw two atoms together and measure how they scatter. You see that for this amplitude to be real, all the particles need to be on-shell or nearly so. If they are not, then the propagator associated with this is small.

A next order contribution to the scattering, representing more than just an improvement on one of the propagators, is



The four external legs always remain present, in any scattering type of diagram that we draw. We do not always want to drag the factor

$$iD_0(k_1)iD_0(k_2)iD_0(k_1-q)iD_0(k_2+q)$$
(9.37)

along in every expression, so we'll modify Feynman rule #3 for $T(k_1,k_2;q)$, and use

3 For each line from spacetime point a to b, except lines connecting to external points, write down an unperturbed propagator $iD_0(b-a)$.

in stead. Then the lowest order approximation of $T(k_1,k_2;q)=ig$. The contribution of the diagram above is

$$T_{(2)}(k,k';q) \propto (-ig)^2 \int \frac{dp}{(2\pi)^4} iD_0(k+k'-p)iD_0(p)$$
 (9.38)

There is a 4-momentum p running around in the loop. This can be freely chosen, so we need to integrate over it, according to Feynman rule #5.

9.6 The trouble with loops

Consider the simplest loop, in the first order correction to D(k):



The 4-momentum q runs around the loop, and we encounter the integral

$$\mathcal{I} = \int \frac{dq}{(2\pi)^4} D(q) = \int \frac{dq}{(2\pi)^4} \frac{1}{q^2 - m^2 + i\varepsilon}$$
(9.39)

Let's split this in energy and 3-momentum integrations,

$$\mathcal{I} = \int \frac{d\omega}{2\pi} \int \frac{d\vec{q}}{(2\pi)^3} \frac{1}{\omega^2 - \vec{q}^2 - m^2 + i\varepsilon}$$
(9.40)

Using $\omega_q = \sqrt{\vec{q}^2 + m^2}$ we can write this as

$$\mathcal{I} = \int \frac{d\vec{q}}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{1}{(\omega - \omega_q + i\varepsilon)} \frac{1}{(\omega + \omega_q - i\varepsilon)}$$
(9.41)

The integration over ω can be performed by contour integration – choose for example a large half circle closing in the upper half of the complex plane. This contains the pole at $\omega = -\omega_q + i\varepsilon$, and we find using the residue theorem

$$\int \frac{d\omega}{2\pi} \frac{1}{(\omega - \omega_q + i\varepsilon)} \frac{1}{(\omega + \omega_q - i\varepsilon)}$$
(9.42)

$$= 2\pi i \lim_{z \to -\omega_q + i\varepsilon} \left[\frac{1}{2\pi} \frac{1}{(\omega - \omega_q + i\varepsilon)} \right] = -\frac{i}{2\omega_q}$$
(9.43)

Hence, we get

$$\mathcal{I} \propto \int \frac{d\vec{q}}{\left(2\pi\right)^3} \frac{1}{\sqrt{\vec{q}^2 + m^2}} \tag{9.44}$$

However, this integral diverges – the integrand goes to zero as $|\vec{q}|^{-1}$, but the integration measure grows as $|\vec{q}|^2$ for $|\vec{q}| \to \infty$. The integral blows up! This reflects the fact that for atoms, the contact potential is just an approximation. Going to very large $|\vec{q}|$ means going to very small distances, and there we know that we should use a real interatomic potential in stead of the delta function $gV(r_1 - r_2)$. Doing things better corresponds to letting g depend on q. We can do this for the exact potential, or try to use a cut-off to regularize the integral. The latter approach assumes that whatever error we make at large q won't matter for the low-energy physics or processes that we try to study. But, whichever approach you take to solving the problem, remember: loops are dangerous.

9.7 Regularization and Renormalization

In quantum field theory³, free fields can be handled exactly, as we have seen above. For interacting fields, perturbation theory leads to an expansion in powers of interaction terms. The computation producedure dictated by perturbative

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 $^{^{3}}$ I found this nice and short discussion on (dimensional) renormalization in a *Physics Today* article (February 2014 issue) by Wolfgang Bietenholz and Lilian Prado. It is suitable to include it here at this point with just a few small notation changes.
quantum field theory seems straightforward, but as we have seen in practice it generates integrals such as

$$\int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + m^2},\tag{9.45}$$

which diverge as the momentum p gets large.

To handle the infinities that a quantum field theory presents, one needs to regularize the integrals – that is, render them finite while preserving the symmetries of the theory or allowing those symmetries to be restored in the final limit in which the regulator is removed. A conceptually simple approach to regularization in to introduce a momentum cutoff Λ to the integrals. The idea is that whatever happens at momenta larger than Λ shouldn't influence the phenomena under investigation at lower energies. But in quantum electrodynamics among other quantum field theories, such a cutoff will not preserve the crucial symmetries.

A better approach is dimensional regularization, in which one begins with an integral in D rather than in four dimensions. For example:

$$\int \frac{d^D k}{(2\pi)^D} \frac{1}{k^2 + m^2} = \int \frac{d^D k}{(2\pi)^D} \int_0^\infty dt \ e^{-(k^2 + m^2)t}$$
$$= \frac{1}{(4\pi)^{D/2}} \int_0^\infty dt \ t^{-D/2} e^{-m^2t}$$
$$= \frac{m^{D-2}}{(4\pi)^{D/2}} \Gamma(1 - D/2)$$
(9.46)

Here the gamma function –the famous generalization of the factorial– is given by

$$\Gamma(z) = \int_{0}^{\infty} d\tau \ \tau^{z-1} e^{-\tau} \tag{9.47}$$

It is well defined for all complex z with a positive real part, and integration by parts gives $\Gamma(z-1) = \Gamma(z)/(z-1)$. The recursion allows the Γ function to be analytically continued over the entire complex plane, except for zero and the negative integers. In particular, in $D = 4 + \varepsilon$ dimensions, the Γ function of equation (9.46) becomes

$$\Gamma(-1 - \varepsilon/2) = \frac{2}{\varepsilon} + \gamma - 1 + \mathcal{O}(\varepsilon)$$
(9.48)

where $\gamma = 0.577...$ is the Euler-Masceroni constant.

In the dimensionally regularized integral, the divergence presented by the perturbation prescription is isolated in the $1/\varepsilon$ term, which, of course, blows up when ε is taken to zero – that is, when one returns to four dimensions.

According to the computational rules for quantum field theories, those divergencies formally contribute to physical quantities such as the mass $m_{\rm physical}$ of a particle. However, physical quantities also recieve contributions governed by so-called bare parameters built into quantum field theories, such as the mass m in the above formulae. For a physical parameter such as $m_{\rm physical}$ to remain finite as ε goes to zero, the appropriate bare parameters must diverge in such a way as to cancel out the $1/\varepsilon$ term arising from the regularization. We did a similar thing for the spring constants and the mass points in our example system: in order to keep the physical mass density and tension of the string finite, these quantities had to go to zero or infinity as ε goes to zero.

Does a given quantum field theory contain enough bare parameters to soak up all the problematic potential divergences and safely allow the regulator (here ε) to approach zero? And will the procedure for canceling divergencies preserve the theorie's crucial symmetries? A theory that can answer yes to both questions is said to be renormalizable. In practice, establishing that a theory is renormalizable can be a very difficult business indeed.

9.8 Spontaneously broken symmetry

9.8.1 Vacuum expectation value

We have looked at Lagrangians of the form

$$\mathcal{L} = \partial_{\mu}\phi^*\partial^{\mu}\phi - V(\phi), \qquad (9.49)$$

with $V(\phi)$ a potential energy for the field, such that global U(1) symmetry is present, such as

$$V(\phi) = m^2 |\phi|^2 + g |\phi|^4, \qquad (9.50)$$

then the ground state (lowest energy field configuration) is given by $\phi = 0$, the particle vacuum. We take g positive, otherwise the field would collapse on itself $(|\phi|^2 \to \infty \text{ obviously makes no sense})$. When we calculate expectation values such as Z or $-i \langle \phi_x \phi_y^* \rangle$, these are calculated with respect to the ground state of the system, so $\phi = 0$.

However, we could also consider potentials of the form

$$V(\phi) = -m^2 |\phi|^2 + g |\phi|^4, \qquad (9.51)$$

as these also conserve global U(1) symmetry. However, the ground state is no longer the state $\phi = 0$, since the lowest energy is achieve for $|\phi|^2 = m^2/(2g)$. There is a nonzero vacuum expectation value (VEV) This can be seen by rewriting the quartic potential as

$$V(\phi) = g\left(|\phi|^2 - \frac{m^2}{2g}\right)^2 - \frac{m^4}{4g}$$
(9.52)

$$\Rightarrow \mathcal{L} = \partial_{\mu}\phi^*\partial^{\mu}\phi - g\left(|\phi|^2 - \frac{m^2}{2g}\right)^2.$$
(9.53)



Figure 9.1: The potential $V(\phi) = -m^2 |\phi|^2 + g |\phi|^4$ (with g > 0) is shaped like a Mexican hat according to Americans and like the bottom of a wine bottle according to the French. All points in the bottom of valley represent possible ground states, nature spontaneously picks one (for example the black dot). In stead of expanding around $\phi = 0$, it is now better to expand around the vacuum expectation value (i.e. the black dot).

In the Lagrangian, we can drop the constant term. Here we something special is going on: there are many possible choices for the ground state: the phase θ can be chosen freely: $\phi_{VEV} = (m/\sqrt{2g}) e^{i\theta}$ This can be seen in figure 9.1: there is a valley in which we can choose freely which point we take. However, once we fix the phase we no longer have U(1) symmetry. Any solution with U(1)symmetry would have $\langle \phi \rangle = 0$, the phase would average out the field even if $\langle |\phi| \rangle \neq 0$. Nature chooses a phase, and hence breaks the U(1) symmetry. The situation is analogous to that of spontaneous magnetization: the direction of the ferromagnetic moment can be chosen freely, but nature picks one choice. This is phenomenon is called *spontaneously broken symmetry*.

The spontaneous breaking of a symmetry is associated with

- a phase transition, from the highly symmetric phase (U(1) in our case) to a phase with lower symmetry. The order parameter that we can assign to the broken symmetry phase is $\langle \phi \rangle$, as it remains zero as long as we are in the highly symmetric phase.
- a Goldstone mode, if the symmetry that we break is a continuous symmetry. This Goldstone mode is a field fluctuation (around the vacuum expectation value) that does not cost energy. In other words, there is an excitation of the field such that the energy of this excitation goes to zero as the wave number k goes to zero.

9.8.2 Goldstone mode

When there is a vacuum expectation value $\phi_{VEV} \neq 0$ it does not make much sense to expand (exponents for example) around $\phi = 0$. You'll need too many terms before the result starts to converge to anything meaningful. The way to proceed is to shift the definition of the field such to the vacuum expectation value, and expand in the neighborhood of ϕ_{VEV} . This is achieved by the *Bogoliubov shift*:

$$\phi(x) = \phi_{VEV} + \chi(x). \tag{9.54}$$

We rewrite the field as a new field $\chi(x) = \chi_R(x) + i\chi_I(x)$ for which $\langle \chi \rangle = 0$. Then we can apply the perturbation techniques of this chapter to this new field. Here ϕ_{VEV} is a constant, independent of x. Let's find the field Lagrangian for the shifted field χ is. We choose a phase $\phi_{VEV} = (m/\sqrt{2g}) e^{i0}$, picking the ground state that lies on the real axis:

$$\phi(x) = \frac{m}{\sqrt{2g}} + \chi_R(x) + i\chi_I(x). \tag{9.55}$$

The kinetic part of the Lagrangian doesn't change when we just add a constant,

$$\partial_{\mu}\phi^{*}\partial^{\mu}\phi = \frac{1}{2}\partial_{\mu}\phi_{R}\partial^{\mu}\phi_{R} + \frac{1}{2}\partial_{\mu}\phi_{I}\partial^{\mu}\phi_{I}$$
$$= \frac{1}{2}\partial_{\mu}\chi_{R}\partial^{\mu}\chi_{R} + \frac{1}{2}\partial_{\mu}\chi_{I}\partial^{\mu}\chi_{I}.$$
(9.56)

What does change, is

$$\begin{aligned} |\phi|^2 &= \phi_R^2 + \phi_I^2 = \left(\frac{m}{\sqrt{2g}} + \chi_R(x)\right)^2 + \chi_I^2(x) \\ &= \frac{m^2}{2g} + \sqrt{\frac{2}{g}} m \chi_R(x) + \chi_R^2(x) + \chi_I^2(x). \end{aligned}$$
(9.57)

Hence

$$-g\left(\left|\phi\right|^{2}-\frac{m^{2}}{2g}\right)^{2} = -g\left(\sqrt{\frac{2}{g}}m\chi_{R}(x)+\left|\chi\right|^{2}\right)^{2}$$
$$=\underbrace{-2m^{2}\chi_{R}^{2}(x)-2\sqrt{2g}m\chi_{R}(x)\left|\chi\right|^{2}-g\left|\chi\right|^{4}}_{\text{mass term interaction terms}}.$$
(9.58)

The only term that is quadratic in the fields (and hence contributes to the free field) is $-2m^2\chi_R^2(x)$. The other terms represent interactions – and now we can again expand the exponent of the action in order to set up a perturbation series to study the effect of these interactions. The entire Lagrangian becomes

$$\mathcal{L} = \left(\frac{1}{2}\partial_{\mu}\chi_{R}\partial^{\mu}\chi_{R} - 2m^{2}\chi_{R}^{2}(x)\right) + \left(\frac{1}{2}\partial_{\mu}\chi_{I}\partial^{\mu}\chi_{I}\right) + \mathcal{L}_{\text{interactions}}$$
(9.59)

The field χ_R is massive (with mass $M = \sqrt{2}m$), and hence it costs a minimum energy Mc^2 to excite a quantum of this field. Such excitations correspond to

the red arrow in figure 9.1, the mass gives curvature to the energy profile. The field χ_I on the other hand is massless, so that $E = \sqrt{\vec{p}^2 + m^2} \rightarrow E = |\vec{p}|$. As the momentum goes to zero, the energy required to make such an excitation also goes to zero. This is the Goldstone mode associated with breaking the U(1) symmetry. It is indicated with a blue arrow in figure 9.1: you do not need to invest energy to walk along the valley of the potential.

9.8.3 Mechanism of Brout, Englert and an Englishman

The existance of a nonzero vacuum expectation value was exploited by Brout, Englert, and Higgs to construct a mechanism whereby massless fields obtain a mass term. For this, they have to introduce a new field (and a new particle), the Brout-Englert-Higgs boson. This has a Lagrangian of the type we used previously:

$$\mathcal{L}_{BEH} = \partial_{\mu}\phi_{H}^{*}\partial^{\mu}\phi_{H} - g_{H}\left(\left|\phi_{H}\right|^{2} - \frac{m_{H}^{2}}{2g_{H}}\right)^{2}.$$
(9.60)

Consider adding this to the Lagrangian of the massless (interacting) scalar field,

$$\mathcal{L}_{\phi} = \partial_{\mu} \phi^* \partial^{\mu} \phi - g \left| \phi \right|^4, \qquad (9.61)$$

as well as including an interaction term between the Brout-Englert-Higgs boson and the massless field,

$$\mathcal{L}_{\text{int}} = -G \left| \phi_H \right|^2 \left| \phi \right|^2. \tag{9.62}$$

The total Lagrangian is $\mathcal{L} = \mathcal{L}_{BEH} + \mathcal{L}_{\phi} + \mathcal{L}_{int}$. If the massless field is a gauge boson, the interaction term can appear simply because of the use of a covariant derivative:

$$\partial_{\mu}\phi_{H}^{*}\partial^{\mu}\phi_{H} \to (\partial_{\mu} + iA_{\mu})\phi_{H}^{*}(\partial^{\mu} - iA^{\mu})\phi_{H}$$
(9.63)

contains an $A_{\mu}A^{\mu}\left|\phi_{H}\right|^{2}=\left\|A\right\|^{2}\left|\phi_{H}\right|^{2}$ term in the Lagrangian.

At low temperatures (when the system goes to the ground state), the U(1) symmetry of \mathcal{L}_{BEH} will be spontaneously broken, resulting in a vacuum expectation value $\phi_{H,VEV} = m_H/\sqrt{2g_H}$. We need to Bogoliubov shift the field in order to study the quantum fluctuations around this expectation value:

$$\phi_H(x) \to \frac{m_H}{\sqrt{2g_H}} + \chi(x).$$
 (9.64)

We have already investigated the effect of this Bogoliubov shift on \mathcal{L}_{BEH} , but now we need to look at the effect on \mathcal{L}_{int} as well. Using (9.57) we get

$$\mathcal{L}_{\text{int}} = -G \left[\frac{m_H^2}{2g_H} + \sqrt{\frac{2}{g_H}} m_H \chi_R + |\chi|^2 \right] |\phi|^2$$

$$= \underbrace{-\frac{Gm_H^2}{2g_H} |\phi|^2}_{\text{mass term for } \phi} \underbrace{-G\sqrt{\frac{2}{g_H}} m_H \chi_R |\phi|^2 - G |\chi|^2 |\phi|^2}_{\text{interaction term}}.$$
(9.65)

The last two terms represent the interaction of the formerly massless field with the quantum fluctuations around the vacuum expectation value of the Brout-Englert-Higgs field. When we freeze out the Brout-Englert-Higgs field (by working at temperatures much much lower than $m_H c^2/k_B$, there are no BEH bosons around to interact with. However, the mass term does not vanish in that limit, we can transfer it to \mathcal{L}_{ϕ} , which becomes

$$\mathcal{L}_{\phi} = \partial_{\mu} \phi^* \partial^{\mu} \phi - M |\phi|^2 - g |\phi|^4$$

with $M = \sqrt{\frac{G}{2g_H}} m_H.$ (9.66)

A mass term has appeared in \mathcal{L}_{ϕ} , and is there even if $\langle \chi \rangle = 0$. This is the mechanism providing the mass to the particles. Apart from m_H , g_H it requires specifying a Yukawa coupling strength G. However, for the gauge bosons, the coupling strength is fixed by the covariant derivative, and it is here that the mechanism can simplify the model by removing the need to fix the masses of the gauge bosons separately.

Chapter 10

Fermionic fields

10.1 Grassmann variables for fermionic fields

10.1.1 The Grassmann algebra

Scalars, spinors (like Dirac), tensors, containing real or complex numbers, don't anticommute. Of course this is because the real and complex numbers don't anticommute. Picking two masspoints on our string we obviously have $\varphi_{\ell}\varphi_{j} = \varphi_{j}\varphi_{\ell}$. However, if we deal with a fermionic field we want these to anticommute since swapping two fermionic mass points should give us a minus sign.

What kind of variables would do that? In fact, you already know an example of anticommuting variables: the eigenvalues of fermionic annihilation or creation operators, $\hat{a}_j |\eta_j\rangle = \eta_j |\eta_j\rangle$. From $\{\hat{a}_j, \hat{a}_\ell\} = 0$ you find that $\eta_j \eta_\ell = -\eta_\ell \eta_j$. Obviously, such η_j 's cannot be elements of \mathbb{R} or \mathbb{C} . We will denote that the η_j 's are Grassmann variables by writing $\eta_j \in \mathbb{G}$, just as we did for the real field by writing $\varphi_j \in \mathbb{R}$.

For these variables, we need to *axiomatically* introduce a new algebra, the **Grassmann** algebra. You may think this is daunting, but remember the time when you were taught that you can never take the square root of a negative number. At some point, someone told you that if you just accept the existence of $\sqrt{-1}$, rules can be found to make things work. Approach the Grassmann variables in the same spirit.

An "algebra" is a mathematical structure – it has at its core a vector space. Vector spaces have an addition (forming a group) and a multiplication by a scalar, such that any linear combination of vectors is again a vector. To make an algebra, we have to add another operation, namely multiplication of two elements. This multiplication should also form a group (except for the fact that the neutral element doesn't have a symmetrical element). Think of matrices: you can add them, multiply them by a scalar, and multiply two matrices. They form an algebra. Also \mathbb{R}^n and \mathbb{C}^n form an algebras, and in fact we have been using these algebra's to make our bosonic fields.

Now we want to make an algebra \mathbb{G}^n , starting with n Grassmann basis vectors $\{\eta_j \in \mathbb{G}\}_{j=1...n}$. Any linear combination of those (such as $c_0+c_1\eta_1+c_2\eta_2$ with c_0, c_1, c_2 complex numbers) is again part of the algebra \mathbb{G}^n . So far, no difference from \mathbb{C}^n . Where it becomes different is that we introduce a new kind of multiplication – one that axiomatically satisfies

$$\forall \eta_a, \eta_b \in \mathbb{G}^n : \eta_a \eta_b = -\eta_b \eta_a, \tag{10.1}$$

so that for any two Grassmann variables (elements of the Grassmann algebra) multiplication anti-commutes. This is non-abelian, but in a very specific way.

Having set down the rule for multiplication, we now need to see where this mathematical spielerei leads us. The first and simplest consequence is that for all η_i in the algebra we have

$$\eta_j^2 = -\eta_j^2 \Leftrightarrow \eta_j^2 = 0. \tag{10.2}$$

Indeed, the only element that is equal to its opposite, is the neutral element for addition: zero.

Functions of Grassmann variables are defined through their Taylor series. For a function depending on only η_{23} we get

$$f(\eta_{23}) = c_0 + c_1 \eta_{23} \tag{10.3}$$

with $c_0, c_1 \in \mathbb{C}$. The Taylor series stops at the linear term since $\eta_{23}^2 = 0$ so all higher powers are also zero. So, there are in a sense way less functions of a grassmann variable than there are of a real variable! That will make derivatives and integrations much easier too. First, what would be the most general function of 2 grassmann variables, say η_8 and η_{13} ? It is

$$f(\eta_8, \eta_{13}) = c_0 + c_1\eta_8 + c_2\eta_{13} + c_3\eta_8\eta_{13} \tag{10.4}$$

with again $c_0, c_1, c_2, c_3 \in \mathbb{C}$. We can generalize this to a function of any $\eta \in \mathbb{G}^n$:

$$f(\eta) = \sum_{n=0}^{25} \sum_{j_1, j_2, \dots, j_n=1}^{25} \frac{1}{n!} \frac{\partial^n f}{\partial \eta_{j_1} \dots \partial \eta_{j_{25}}} \eta_{j_1} \dots \eta_{j_n}$$
(10.5)

(here for our simpleversum with 25 spacetime points) where the product of η 's should be such that each variable appears at most once. And of course the order matters – moreover we now need to specify what it means to derive with respect to a Grassmann variable.

Derivatives with respect to Grassman variables are particularly simple, and defined by

$$\partial_{\eta_j} \eta_\ell = \delta_{j\ell} \tag{10.6}$$

Note that ∂_{η_j} also anticommutes, so

$$\partial_{\eta_1}(\eta_2\ldots) = -\eta_2 \partial_{\eta_1}(\ldots)$$

For example, taking the derivative of the function defined in expression 10.4 is

$$\partial_{\eta_{13}} f(\eta_8, \eta_{13}) = c_2 + c_3 \partial_{\eta_{13}} \left(\eta_8 \eta_{13} \right) = c_2 - c_3 \eta_8 \partial_{\eta_{13}} \left(\eta_{13} \right) = c_2 - c_3 \eta_8 \quad (10.7)$$

Integration is completely defined by

$$\int d\eta_j = 0 \quad \text{and} \quad \int d\eta_j \eta_j = 1 \tag{10.8}$$

Hence

$$\int d\eta_j \eta_\ell = \delta_{j\ell} \tag{10.9}$$

and we also have

$$\int d\eta_j \left(\eta_\ell \dots\right) = -\eta_\ell \int d\eta_j \left(\dots\right). \tag{10.10}$$

So in fact taking the derivative is identical to integrating! Indeed,

$$\int d\eta_{13} f(\eta_8, \eta_{13}) = (c_0 - c_1 \eta_8) \int d\eta_{13} + (c_2 - c_3 \eta_8) \int d\eta_{13} \eta_{13}$$

= $c_2 - c_3 \eta_8.$ (10.11)

Integrals with respect to Grassmann variables are also called *Berezin integrals*. Analysis of functions of Grassman variables is much simpler that complex analysis, once you get the hang to it!

10.1.2 Grassmann path integrals

Let's start with a simple Gaussianish integral:

$$\int d\eta_j \int d\eta_\ell \exp\left\{-a\eta_j\eta_\ell\right\}$$
(10.12)

with $a \in \mathbb{C}$. Note that the order of integrations is crucial,

$$\int d\eta_j \int d\eta_\ell = -\int d\eta_\ell \int d\eta_j \tag{10.13}$$

The exponential is defined through its Taylor series,

$$\exp\left\{-a\eta_j\eta_\ell\right\} = 1 - a\eta_j\eta_\ell \tag{10.14}$$

Hence

$$\int d\eta_j \int d\eta_\ell \exp\left\{-a\eta_j\eta_\ell\right\} = \int d\eta_j \int d\eta_\ell \left(1 - a\eta_j\eta_\ell\right)$$
$$= -a \int d\eta_j \int d\eta_\ell \eta_j \eta_\ell$$
$$= +a \int d\eta_j \eta_j \int d\eta_\ell \eta_\ell$$
$$= +a \qquad (10.15)$$

Note if you integrate over η_j and η_ℓ , this picks out terms in the Taylor expansion that contain both η_j and η_ℓ . Note also that *a* now comes in the numerator, for a complex field the Gaussian integral (see expression (7.38)) is proportional to 1/a. Now we can go to more than just two variables, and populate spacetime with Grassmann variables in each spacetime point.

When we have a scalar field representing a boson, we use complex scalars. In each point in space we have two degrees of freedom, ϕ and ϕ^* . Without complexvalued fields, creation and annihilation would be the same, and propagators would not have an arrow. Indeed, $D(x - y) = -i \langle \phi(x) \phi^*(y) \rangle$ is not the same as D(y - x), but that difference vanishes when we have real fields. Similarly, when we switch to Grassmann variables we want to have two degrees of freedom in each spacetime point, ψ and $\overline{\psi}$. Quadratic action functionals for Grassmann fields then look like

$$Z = \int \mathcal{D}\psi \exp\left\{\sum_{x,y} \bar{\psi}_x A_{xy} \psi_y\right\}$$
(10.16)

Since also the *order of the integrals* matter, we must adopt a convention here, and set

$$\int \mathcal{D}\psi = \left(\int d\bar{\psi}_1 \int d\psi_1\right) \left(\int d\bar{\psi}_2 \int d\psi_2\right) \dots$$
(10.17)

If you swap any two integrals, there's going to be a minus sign. If you swap integrals for two spacetime points (1 and 2 for example), this corresponds to swapping a pair of individual integrations over Grassmann variables, and there is no sign change.

Let's look at a simple example to see how this works out. Take

$$S = \bar{\psi}_1 a_{11} \psi_1 + \bar{\psi}_1 a_{12} \psi_2 + \bar{\psi}_2 a_{21} \psi_1 + \bar{\psi}_2 a_{22} \psi_2 \tag{10.18}$$

Hence,

$$e^{-S} = 1 + \bar{\psi}_1 a_{11} \psi_1 + \bar{\psi}_1 a_{12} \psi_2 + \bar{\psi}_2 a_{21} \psi_1 + \bar{\psi}_2 a_{22} \psi_2 + \frac{1}{2} \left(\bar{\psi}_1 a_{11} \psi_1 + \bar{\psi}_1 a_{12} \psi_2 + \bar{\psi}_2 a_{21} \psi_1 + \bar{\psi}_2 a_{22} \psi_2 \right)^2$$
(10.19)

We do not need to go to higher orders of the expansion, since they all contain squares of one or another Grassmann variable. In fact, most terms from the

second order term also vanish: only those terms that have all different ψ 's remain:

$$e^{-S} = 1 + \bar{\psi}_1 a_{11} \psi_1 + \bar{\psi}_1 a_{12} \psi_2 + \bar{\psi}_2 a_{21} \psi_1 + \bar{\psi}_2 a_{22} \psi_2 + (\bar{\psi}_1 a_{11} \psi_1) (\bar{\psi}_2 a_{22} \psi_2) + (\bar{\psi}_1 a_{12} \psi_2) (\bar{\psi}_2 a_{21} \psi_1). \quad (10.20)$$

Integrating and differentiating is the same, so the constant term will vanish, and terms that do not have *all* the Grassmann variables will also vanish. For example, the term $-\bar{\psi}_1 a_{11}\psi_1$ vanishes if you integrate it with respect to ψ_2 . Hence,

$$\int \mathcal{D}\psi e^{-S} = \int d\bar{\psi}_1 \int d\psi_1 \int d\bar{\psi}_2 \int d\psi_2 \ (\bar{\psi}_1 a_{11}\psi_1) \ (\bar{\psi}_2 a_{22}\psi_2) \\ + \int d\bar{\psi}_1 \int d\psi_1 \int d\bar{\psi}_2 \int d\psi_2 \ (\bar{\psi}_1 a_{12}\psi_2) \ (\bar{\psi}_2 a_{21}\psi_1) (10.21)$$

In the first line, the integrations are in the same order as the factors in the integrand, $\bar{\psi}_1\psi_1\bar{\psi}_2\psi_2$. In the second line, there has been one swap $\psi_1 \leftrightarrow \psi_2$ to obtain $\bar{\psi}_1\psi_2\bar{\psi}_2\psi_1$, leading to a minus sign. We get

$$\int \mathcal{D}\psi e^{-S} = a_{11}a_{22} - a_{12}a_{21} = \det \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}.$$
 (10.22)

In general (if you feel like doing a lot of bookkeeping it is not intrinsically difficult to show that)

$$Z = \int \mathcal{D}\psi \exp\left\{\sum_{x,y} \bar{\psi}_x A_{xy} \psi_y\right\} = \det\left(A\right)$$
(10.23)

Remember that for bosons $Z=1/\det(A)$, the result for the fermions seems to be... the inverse.

10.1.3 Fermionic Green's function

Whatever we can do for bosons, we can do for fermions! We want to see how the integral

$$Z^{\text{boson}}(J) = \int \mathcal{D}\phi \exp\left\{-i\sum_{x,y} \phi_x^* A_{xy} \phi_y + i\sum_x \left(J_x \phi_x^* + J_x^* \phi_x\right)\right\}$$
$$= Z^{\text{boson}}(0) \exp\left\{i\sum_{x,y} J_x^* A_{xy}^{-1} J_y\right\}$$
(10.24)

generalizes. That is, we want to find

$$Z^{\text{fermion}}(J) = \int \mathcal{D}\psi \exp\left\{i\sum_{x,y} \bar{\psi}_x A_{xy}\psi_y + i\sum_x \left(\bar{\psi}_x J_x + \bar{J}_x\psi_y\right)\right\}$$
(10.25)

Note that the source terms must now also be Grassmann variables! To see the structure of the result, we do the integrations for the simpler case

$$z_J = \int d\bar{\psi} \int d\psi \exp\left\{a\bar{\psi}\psi + \bar{\psi}J + \bar{J}\psi\right\}$$
(10.26)

Remember that the multiplication –even the weirdo anticommuting one– is distributive over the addition, so you can again complete the squares (keeping the order of the variables):

$$z_J = \int d\bar{\psi} \int d\psi \exp\left\{a\left(\bar{\psi} + \bar{J}/a\right)\left(\psi + J/a\right) - \bar{J}J/a\right\}$$
(10.27)

A linear combination of Grassmann variables is still a Grassmann variable $\eta=\psi-J/a$, so we get back the gaussian integral

$$z_J = z_0 \exp\left\{-\bar{J}J/a\right\} \tag{10.28}$$

where $z_0 = a$. Multiplying a, J, \overline{J} by *i* gives an overall factor *i* in the exponent. Going back to matrices, we get

$$Z^{\text{fermion}}(J) = Z^{\text{fermion}}(0) \exp\left\{-i\sum_{x,y} \bar{J}_x A_{xy}^{-1} J_y\right\}$$
(10.29)

so that for Z(J) there is a full analogy with the bosonic case – however now order matters! If we calculate the fermion pair correlation

$$\tilde{G}(x,y) = -i \left\langle \psi_x \bar{\psi}_y \right\rangle = -i \left. \frac{\partial}{\partial i J_x} \frac{\partial}{\partial i \bar{J}_y} \frac{Z^{\text{fermion}}(J)}{Z^{\text{fermion}}(0)} \right|_{J=0}$$
(10.30)

$$= i \frac{\partial}{\partial J_x} \frac{\partial}{\partial \bar{J}_y} \exp\left\{-i \sum_{u,v} \bar{J}_u A_{uv}^{-1} J_v\right\}$$
(10.31)

The only term that contributes is

$$\tilde{G}(x,y) = i(-i)\frac{\partial}{\partial J_x}\frac{\partial}{\partial \bar{J}_y}\left(\bar{J}_y A_{yx}^{-1} J_x\right) = \frac{\partial}{\partial J_x}A_{yx}^{-1} J_x = A_{yx}^{-1}$$
(10.32)

So, the pair expectation value is still A_{yx}^{-1} , the inverse of A or, in case A is a linear operator, the Green's function corresponding to that linear operator. Note that now $G(x, y) \neq G(y, x)$, whereas for bosons D(x, y) = D(y, x). We'll get back to this point later, as we need to introduce a "standard ordering". But first, the good news that we get from the above calculation:

Hence, in practice, when doing calculation with Feynman diagrams using fermionic Green's functions for propagators, it does not matter that the actual field variables are Grassmannian!

10.2 The Dirac field

When a bosonic field consists of multiple components, we have imposed relations between these components by saying how they transform under for rotations and Lorentz boosts. This has led us to vector and tensor fields. For fermions, this will be different – as we know from the spin-statistics theorem, fermions behave differently under rotation: you have to turn them around by 4π before you get the same sign. We will see that fermionic multicomponent fields arrange themselves in spinors, the simpest of which is the Dirac spinor. Of course, you are not obliged to use Dirac spinors to set up a theoretical model involving fermions – this is only needed when you impose Lorentz invariance!

10.2.1 The Lorentz group

The Lorentz algebra

The Lorentz boosts do not form a group – the rotations have to be added to this set in order to obtain a group. The generators of rotations in the yz, xzand xy plane (namely J_x, J_y, J_z) and the generators of boosts in along x, y, z(namely K_x, K_y, K_z) have the following Lie algebra:

$$[J_j, J_k] = i\varepsilon_{jk\ell} J_\ell, \tag{10.33}$$

$$[J_i, K_k] = i\varepsilon_{ik\ell} K_\ell, \tag{10.34}$$

$$[K_j, K_k] = -i\varepsilon_{jk\ell} J_\ell, \tag{10.35}$$

where $\varepsilon_{jk\ell}$ is the Levy-Civita tensor, equal to 1 for even permutations of x, y, z, -1 for odd permutations, and 0 for other combinations. This extended group is called SO(3, 1), denoting the fact that there are three spatial and one time dimension. Rotating in a plane of two spatial dimensions gives a usual rotation (with cos and sin as matrix elements for the transformation). The Lorentz boosts can be though of as "rotations" in a plane with one time and one spatial dimension, where now we have cosh and sinh in the matrix element (cf. expression (4.13)) – this is like cos and sin with an imaginary angle, the rapidity ϑ . The fact that when the time dimension is envolved we get hyperbolic functions rather than goniometric makes time "special", and distinguishes SO(4) from SO(3, 1).

The rotations in spatial planes are parametrized by three angles $\theta_x, \theta_y, \theta_z$. The boosts are characterized by three more continuous parameters (the rapidities) $\vartheta_x, \vartheta_y, \vartheta_z$, where $\vartheta_\ell = \operatorname{arctanh}(v_\ell/c)$. Any transformation Λ of the Lorentz group is identified by these six parameters, and can be written down using the generators as follows

$$\Lambda = \exp\left\{i\mathbf{J}\cdot\boldsymbol{\theta} + i\mathbf{K}\cdot\boldsymbol{\vartheta}\right\}$$
(10.36)

where $\mathbf{J} \cdot \boldsymbol{\theta} = J_x \theta_x + J_y \theta_y + J_z \theta_z$ and similarly for $\mathbf{K} \cdot \boldsymbol{\vartheta}$. If we have a collection of N objects transforming among each other when subject to the Lorentz group, we need to find the corresponding N dimensional representation (which may be decomposed in irreducible representations).

Left- and right-handed Weyl spinors

The crucial observation to set up representations of this group is that the algebra falls apart in two independent sets of commutating quantities if we form the combinations

$$\mathbf{J}_{\pm} = \frac{1}{2} \left(\mathbf{J} \pm i \mathbf{K} \right), \qquad (10.37)$$

$$\Leftrightarrow \begin{cases} \mathbf{J} = \mathbf{J}_{+} + \mathbf{J}_{-} \\ \mathbf{K} = -i \left(\mathbf{J}_{+} - \mathbf{J}_{-} \right) \end{cases}$$
(10.38)

with $\ell = x, y, z$. Indeed, you can verify that

$$[J_{+,j}, J_{+,k}] = i\varepsilon_{jk\ell}J_{+,\ell} \tag{10.39}$$

$$[J_{-,i}, J_{-,k}] = i\varepsilon_{ik\ell}J_{-,\ell} \tag{10.40}$$

$$[J_{-,j}, J_{-,k}] = i\varepsilon_{jk\ell}J_{-,\ell}$$
(10.40)

$$[J_{-,j}, J_{+,k}] = 0$$
(10.41)

The first two lines mean that the J_+ 's and the J_- 's separately form an angular momentum (SU(2)) algebra! We can use our knowledge of the representations of the angular momentum on \mathbf{J}_+ and \mathbf{J}_- . Angular momentum representations are labeled by half-integers j = 0, 1/2, 1, 3/2, 2, ... with respective dimension 2j + 1, i.e. consisting of 2j + 1 objects ψ_m with m = -j, ..., j that transform into each other according to SU(2). It follows immediately that:

- The representations of the Lorentz algebra $SO(3,1) = SU(2) \otimes SU(2)$ will be labeled (j_+, j_-) with two half-integers j_+ and j_- taking on values $0, 1/2, 1, 3/2, \dots$
- The dimension of the respresentation (j_+, j_-) is $(2j_+ + 1)(2j_- + 1)$. This means the representation (j_+, j_-) consists of $(2j_+ + 1)(2j_- + 1)$ objects $\psi_{m_{\pm},m_{\pm}}$ with $m_{\pm} = -j_{\pm},...,j_{\pm}$.
- The generator of rotations **J** is related to \mathbf{J}_+ and \mathbf{J}_- by $\mathbf{J} = \mathbf{J}_+ + \mathbf{J}_-$. Therefore, by the usual addition of angular momenta in quantum mechanics, the representation (j_+, j_-) will have all possible spin j in integer steps between $|j_+ - j_-|$ and $j_+ + j_-$.

The lowest dimensional few representations SO(3,1) are (0,0), (1/2,0), (0,1/2), $(1/2, 1/2), (1, 0), (0, 1), \dots$ Clearly the (0, 0) representation are the Lorentz scalars. The 4-dimensional representation (1/2, 1/2) is the Lorentz vector (one combination, the norm, is a scalar, leaving three degrees of freedom that transform as j = 1). To figure out what we need for fermionic objects we need the famous spin-statistics theorem:

If the spin $j_+ + j_-$ is even, the objects must obey Bose symmetry, whereas if the spin $j_+ + j_-$ is odd, they must obey Fermi symmetry.

10.2. THE DIRAC FIELD

This means at first sight that the simplest representation for a fermion must be either (1/2, 0) or (0, 1/2). In each case, we need at least two (Grassmannian) components for the fermion field. Let's denote these components as *left-handed* and right-handed Weyl spinors, for reasons that will become clear soon enough:

$$\Psi_L = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \in (1/2, 0) \quad \text{and} \quad \Psi_R = \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix} \in (0, 1/2) \quad (10.42)$$

From the "1/2" It is clear that we will need the two-dimensional representations of the angular momentum group. These are obviously generated by the Pauli matrices, and from (10.38)

$$(1/2,0): \begin{cases} J_{\ell,+} \to \sigma_{\ell}/2 \\ J_{\ell,-} \to 0 \end{cases} \Rightarrow \begin{cases} J_{\ell} = \frac{1}{2}\sigma_{\ell} \\ K_{\ell} = -\frac{i}{2}\sigma_{\ell} \end{cases}$$
(10.43)

and

$$(0,1/2): \begin{cases} J_{\ell,+} \to 0\\ J_{\ell,-} \to \sigma_{\ell}/2 \end{cases} \Rightarrow \begin{cases} J_{\ell} = \frac{1}{2}\sigma_{\ell}\\ K_{\ell} = +\frac{i}{2}\sigma_{\ell} \end{cases}$$
(10.44)

Let's first investigate $\Psi_L \in (1/2, 0)$. The zero in (1/2, 0) means that when $J_{-,\ell} = (J_\ell - iK_\ell)/2$ acts on the two objects ψ_1, ψ_2 , nothing changes (i.e. they behave as scalars). However, when $J_{+,\ell} = (J_\ell + iK_\ell)/2$ acts on these objects, they get mixed up according to the two-dimensional representation for the angular momentum, i.e. the Pauli matrices:

$$\Lambda_L \Psi_L = \exp\left\{i\mathbf{J}\cdot\boldsymbol{\theta} + i\mathbf{K}\cdot\boldsymbol{\vartheta}\right\}\Psi_L$$

=
$$\exp\left\{i\frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta} + \frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\vartheta}\right\}\Psi_L \qquad (10.45)$$

Analogously, the two Grassmann objects in $\Psi_R \in (0, 1/2)$ get scrambled up under Lorentz transformations according to

$$\Lambda_R \Psi_R = \exp\left\{i\frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta} - \frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\vartheta}\right\}\Psi_R \tag{10.46}$$

The difference is that the rapidity (and hence the momentum) has switched sign with respect to the spin σ . For the left-handed spinor, boosting leads to a momentum anti-parallel to the spin, whereas for the right-handed spinor Lorentz boosting leads to a momentum parallel to the spin. The two components are also called "chiral" components (as left and right hand are each other's mirror image, i.e. differ in "chirality").

Including parity

So which one do we choose as our simplest Lorentz-invariant fermion ? The one transforming according to (1/2, 0) or to (0, 1/2) ? That depends on what we observe in nature... and what additional symmetry requirements we impose. You could demand, on top of Lorentz invariance, also parity invariance. That means the physics doesn't change if we let $\vec{x} \to -\vec{x}$ (and consequently $\vec{p} \to -\vec{p}$). Doing the parity transformation doesn't change J_{ℓ} , but it changes the sign of K_{ℓ} . Hence, under parity $J_{-,\ell} \longleftrightarrow J_{+,\ell}$! If we want to include parity the simplest fermion must contain all four components

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}, \tag{10.47}$$

This is called *the Dirac spinor* (in the chiral or Weyl representation). It transforms as $(1/2, 0) \oplus (0, 1/2)$, i.e. with generators for rotations the 4x4 matrices

$$\mathbf{J} \to \begin{pmatrix} \boldsymbol{\sigma}/2 & 0\\ 0 & \boldsymbol{\sigma}/2 \end{pmatrix}$$
(10.48)

and for boosts the 4×4 matrices

$$\mathbf{K} \to \begin{pmatrix} -i\boldsymbol{\sigma}/2 & 0\\ 0 & +i\boldsymbol{\sigma}/2 \end{pmatrix}$$
(10.49)

so that

$$\Lambda \Psi = \exp\left\{i\mathbf{J} \cdot \boldsymbol{\theta} + i\mathbf{K} \cdot \boldsymbol{\vartheta}\right\} \Psi \tag{10.50}$$

To perform the parity transformation we need to let the matrix

$$\gamma^{0} = \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \hline 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$
(10.51)

act on Ψ , to swap the upper and lower two components. Using a "parity transform" matrix

$$\gamma^5 = \left(\begin{array}{cc} \mathbb{I} & 0\\ 0 & -\mathbb{I} \end{array}\right) \tag{10.52}$$

we can construct two other projection operators

$$P_L = \frac{1}{2} \left(1 + \gamma^5 \right)$$
 (10.53)

$$P_R = \frac{1}{2} \left(1 - \gamma^5 \right) \tag{10.54}$$

that project out Ψ_L and Ψ_R .

Note that nature breaks parity symmetry! So, in the standard model, it is not necessary to treat the left- and right-handed components in the same way. Indeed, they do not even need to occur both: it was long thought that there are only left-handed neutrino's existed, until observations in 2014 from X-ray spectra of far-away galaxies hinted that also the right-handed neutrino (the socalled "sterile neutrino") might exist and be a candidate for dark matter¹. As it seems to be the weak nuclear force that violates parity, if we have a theory that does not include this force (such as quantum electrodynamics), we need to use all four fields, and combine them into the spinors as outlined above.

10.2.2 The Dirac equation

Parity has forced us to have a 4-component spinor, but we know on the other hand that the (nonrelativistic) electron has only two physical degrees of freedom. We can find those by going to the rest frame, and project out the components of $\Psi(p_r)$ where p_r is the rest frame momentum $p_r = (m, \vec{0})$. The two chiral components differ only by the way they react to a boost: the momentum of the boost changes sign. So, in the rest frame this should not make a difference, and $\Psi_L = (\psi_1, \psi_2)$ should be equal to $\Psi_R = (\psi_3, \psi_4)$. A projection for which $\Psi_L - \Psi_R = 0$ holds is

$$P = \frac{1}{2} \left(1 - \gamma^0 \right) \Psi = \begin{pmatrix} \mathbb{I} & -\mathbb{I} \\ -\mathbb{I} & \mathbb{I} \end{pmatrix} \begin{pmatrix} \Psi_L \\ \Psi_R \end{pmatrix}.$$
(10.55)

Saying that $\Psi_L(p_r) - \Psi_R(p_r) = 0$ is true, is equivalent to imposing the equation

$$(1-\gamma^0)\Psi(p_r)=0$$

Hence, our rest frame fermionic field $\Psi(p_r)$ is actually characterized just by two components,

$$\left(\psi_{\uparrow},\psi_{\downarrow}\right) = \left(\frac{\psi_1 - \psi_3}{2}, \frac{\psi_2 - \psi_4}{2}\right). \tag{10.56}$$

They are commonly designated as the *spin-up* and *spin-down* components of the spin-1/2 fermion.

What equation should be satisfied in general, when we are not in the rest frame? We can easily find this with a Lorentz boost acting on $\Psi(p_r)$. We know how to perform boosts, as we know the generators for them. With $\vartheta_x, \vartheta_y, \vartheta_z$ as rapidities such that $\vartheta_x = \operatorname{arctanh}(v_x/c)$, the transformation acting on the rank 4 column $\Psi(p_r)$ is represented by (10.50) with $\theta = 0$, so that

$$\Psi(p) = \Lambda \Psi(p_r) \tag{10.57}$$

$$\Rightarrow \Psi(p) = \exp\left\{-i\mathbf{K}\cdot\boldsymbol{\vartheta}\right\}\Psi(p_r) \tag{10.58}$$

¹References: Bulbul *et al.*, arxiv.org/abs/1402.2301 and Boyarsky *et al.*, arxiv.org/abs/1402.4119v1.

with

$$i\mathbf{K}\cdot\boldsymbol{\vartheta} = \begin{pmatrix} -\frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\vartheta} & 0\\ 0 & +\frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\vartheta} \end{pmatrix}$$
(10.59)
$$= \frac{1}{2} \begin{pmatrix} -\vartheta_z & -\vartheta_x + i\vartheta_y & 0 & 0\\ -\vartheta_x - i\vartheta_y & \vartheta_z & 0 & 0\\ 0 & 0 & \vartheta_z & \vartheta_x - i\vartheta_y\\ 0 & 0 & \vartheta_x + i\vartheta_y & -\vartheta_z \end{pmatrix} (10.60)$$

a 4×4 matrix. The equation

$$(\gamma^0 - 1) \Psi(p_r) = 0$$
 (10.61)

becomes

$$e^{i\mathbf{K}\cdot\boldsymbol{\vartheta}}\left(\gamma^{0}-1\right)\Psi(p_{r})=0$$

$$\Leftrightarrow \quad \left(e^{i\mathbf{K}\cdot\boldsymbol{\vartheta}}\gamma^{0}e^{-i\mathbf{K}\cdot\boldsymbol{\vartheta}}-1\right)e^{i\mathbf{K}\cdot\boldsymbol{\vartheta}}\Psi(p_{r})=0 \tag{10.62}$$

Introducing the notation

$$\gamma^{\mu} p_{\mu} / m = e^{i\mathbf{K}\cdot\boldsymbol{\vartheta}} \gamma^{0} e^{-i\mathbf{K}\cdot\boldsymbol{\vartheta}} \tag{10.63}$$

we get the famous Dirac equation

$$(\gamma^{\mu}p_{\mu} - m)\Psi(p) = 0$$
(10.64)

All you need to compute are the matrices γ^1, γ^2 and γ^3 (we already have γ^0), resulting from boosts in the x, y, z directions, respectively. Going back from reciprocal space to real space with $p_{\mu} \leftrightarrow i \partial_{\mu}$, this becomes

$$(i\gamma^{\mu}\partial_{\mu} - m)\Psi(x) = 0$$
(10.65)

As you may very well guess, the matrices γ^{μ} are the gamma matrices that you obtained in the usual derivation of the Dirac equation.

Feynman introduced the slash notation to indicate a product of a four-vector and the gamma matrices,

$$\gamma^{\mu}A_{\mu} = A \tag{10.66}$$

In particular we have

$$\gamma^{\mu}\partial_{\mu} = \not \partial \tag{10.67}$$

and we will use this notation in our notes, writing the Dirac equation as

$$(i\partial - m)\Psi(x) = 0. \tag{10.68}$$

10.2.3 Gamma matrices

You can compute the gamma matrices from equation (10.63). Rather than doing that, we will follow the historical derivation of the Dirac equation, just to remind you of your course of advanced quantum mechanics. In that course, you have encountered the Dirac equation as an attempt to modify the Schrödinger equation so that it becomes compatible with special relativity. The Schrödinger equation obviously does not treat time and space the same, since it uses different orders in the derivatives,

$$\left[\left(i\hbar\partial_t \right) - \left(-i\hbar\vec{\nabla} \right)^2 \right] \psi = E\psi \tag{10.69}$$

for an energy mc^2 , this is

$$\left[(i\partial_{ct}) + \vec{\nabla}^2 \right] \psi = \left(\frac{mc}{\hbar} \right)^2 \psi$$

The combination $\hbar/(mc)$ is the Compton length. The simplest way to make this covariant, is to raise the order of the time derivative. That way (and set $\hbar = c = 1$) you obtain the Klein-Gordon equation,

$$\left[-\partial_t^2 + \vec{\nabla}^2\right]\psi = m^2\psi \Leftrightarrow \left(\Box + m^2\right)\psi = 0 \tag{10.70}$$

$$\Rightarrow E^{2} = \bar{p}^{2} + m^{2} \ (\Leftrightarrow \ p^{2} - m^{2} = 0) \tag{10.71}$$

This simple trick is a great success since it is compatible with the fundamental energy equation of special relativity just plug in $\psi = e^{ikx} = e^{iEt/\hbar - i\vec{p}\vec{x}/\hbar}$ to see that). The downside of it (as seen at the time) is that in principe it also allows for negative energy solutions – you could write it as. The other way to make the Schrödinger equation covariant is by reducing the order of the spatial derivative, obtaining an equation with only first derivatives

$$(i\gamma^{\mu}\partial_{\mu} - m)\Psi = 0$$
(10.72)

Dirac may have been thinking: I need to take the "square root" of $p^2 - m^2 = 0$ by setting it equal to (p - m) (p + m) = 0 and selecting p - m = 0 as the positive energy solution, and then replacing p as usual by $i\partial$. That didn't work out with the indices of the momentum four-vector... you need to introduce matrices γ^{μ} for it to have a chance to work out. Now the trick is to choose the coefficients γ^{μ} such that the fundamental energy equation of special relativity is satisfied. Since the Dirac equation is much like a "square root" of the Klein-Gordon equation, p - m, if we multiply it by p + m, we should get back to Klein-Gordon:

$$(i\gamma^{\mu}\partial_{\mu} - m)(i\gamma^{v}\partial_{v} + m)\Psi = 0$$

$$\Leftrightarrow \quad (\gamma^{\mu}\gamma^{\nu}\partial_{\mu}\partial_{v} + m^{2})\Psi = 0$$
(10.73)

Of course, the order of the derivatives doesn't matter. Swapping them around and re-indexing you can see that this equation is equivalent to

$$\Leftrightarrow \left(\frac{1}{2}\left\{\gamma^{\mu},\gamma^{\nu}\right\}\partial_{\mu}\partial_{\nu}+m^{2}\right)\Psi=0$$
(10.74)

with $\{\gamma^{\mu}, \gamma^{\nu}\} = \gamma^{\mu}\gamma^{\nu}$ the anti-commutator. In order to get the Klein-Gordon equation $(\partial_{\mu}\partial^{\mu} + m^2) \psi = 0$, we need

$$\{\gamma^{\mu}, \gamma^{\nu}\} = 2g^{\mu\nu} \tag{10.75}$$

so that the metric can pump the v index up. Note that the right hand side is the number $2g^{\mu\nu}$ for a given μ, ν , multiplied by the unit matrix. There is more than one possible solution. One is the Weyl representation,

$$\gamma^{0} = \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \hline 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$
(10.76)

The $\gamma^1, \gamma^2, \gamma^3$ matrices are defined with the Pauli matrices $\sigma_x, \sigma_y, \sigma_z$:

$$\gamma^{1} = \begin{pmatrix} 0 & \sigma_{x} \\ -\sigma_{x} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ \hline 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$
(10.77)

$$\gamma^{2} = \begin{pmatrix} 0 & \sigma_{y} \\ -\sigma_{y} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ \hline 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}$$
(10.78)

$$\gamma^{3} = \begin{pmatrix} 0 & \sigma_{z} \\ -\sigma_{z} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & | 1 & 0 \\ 0 & 0 & 0 & -1 \\ \hline -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$
(10.79)

The four matrices γ^{μ} transform like 4-vectors under the Lorentz transformation, in the sense that $\gamma^{\nu} = L^{\nu}_{.\mu} \gamma^{\mu}$. There's a fifth gamma matrix, anticommuting with all others $\{\gamma^5, \gamma^{\mu}\} = 0$, and given by

$$\gamma^{5} = i\gamma^{0}\gamma^{1}\gamma^{2}\gamma^{3} = \begin{pmatrix} -\mathbb{I} & 0\\ 0 & \mathbb{I} \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ \hline 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1 \end{pmatrix}$$
(10.80)

The Dirac equation, $(i\partial - m)\Psi = 0$, can of course be Fourier transformed – just substitute a plane wave $\Psi(x) \to \Psi(p)e^{ipx}$ and you find

$$\left(\not p + m\right)\Psi(p) = 0 \tag{10.81}$$

The fact that we need to use 4×4 matrices implies that Ψ contains four components, which for a fermionic field become *four grassmann variables*, that

we can arrange in a column vector. The adjoint vector is not just the row vector with the complex conjugates (Ψ^{\dagger}) , but it is defined by

$$\bar{\Psi} = \Psi^{\dagger} \gamma^5 \tag{10.82}$$

since $(\gamma^{\mu})^{\dagger} = \gamma^5 \gamma^{\mu} \gamma^5$. As mentioned before, there are many 4×4 matrices that do the trick (they are all related by unitary transformations). A commonly used other set is the Dirac representation, where we use $-\gamma^5$ in stead of γ^0 (and γ^5 becomes $-\gamma^0$). The Dirac and Weyl representation have each their advantage.

• Weyl: The top two components of Ψ are the left-handed spinor Ψ_L , and the bottom two are the right handed spinor Ψ_R . These are projected out by $P_L = (1 - \gamma^5)/2$ and $P_R = (1 + \gamma^5)/2$ respectively. The Weyl representation is handy in the relativistic limit (*m* small) since then the Dirac equation is approximately $p\Psi = 0$ with

$$p = \begin{pmatrix} 0 & p_0 - \vec{p} \cdot \vec{\sigma} \\ p_0 + \vec{p} \cdot \vec{\sigma} & 0 \end{pmatrix}$$
(10.83)

the top two components separate from the bottom two. Moreover, for the top two we have $-\vec{p}\cdot\vec{\sigma}$ in the field equation, so that the momentum and the spin for Ψ_L are parallel, whereas for the Ψ_R they are antiparallel.

• Dirac: The top two components of Ψ represent the usual particle spin up and spin down components, whereas the bottom two components represent the corresponding antiparticle.

10.3 Dirac Lagrangian

10.3.1 Free field action

The Dirac equation is the classical field equation corresponding to the Lagrangian

$$\mathcal{L}(\psi,\partial_{\mu}\psi) = \bar{\psi}_{x} \left(i\gamma^{\mu}\partial_{\mu} - m\right)\psi_{x} = i\gamma^{\mu}\bar{\psi}_{x}\partial_{\mu}\psi_{x} - m\bar{\psi}_{x}\psi_{x}$$
(10.84)

Indeed, using our rules for derivatives of grassmann variables:

$$\frac{\partial \mathcal{L}}{\partial \psi_x} = +m\bar{\psi}_x \tag{10.85}$$

$$\frac{\partial \mathcal{L}}{\partial \bar{\psi}_x} = +i\gamma^\mu \partial_\mu \psi_x - m\psi_x \tag{10.86}$$

and since $\partial_{\mu}\psi$ is just a linear combination of Grassmann variables at different spacetime positions, it is also a Grassmann variable,

$$\frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu}\psi\right)} = -i\bar{\psi}_{x}\gamma^{\mu} \tag{10.87}$$

$$\frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu} \bar{\psi}\right)} = 0 \tag{10.88}$$

Note that $\bar{\psi}_x$ is a row vector with four components, so it has to be on the left of the 4 by 4 matrix γ^{μ} . Hence the field equations are

$$\partial_{\mu} \frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu} \bar{\psi}_{x}\right)} = \frac{\partial \mathcal{L}}{\partial \bar{\psi}_{x}} \Leftrightarrow \left(i \not \partial - m\right) \psi_{x} = 0 \tag{10.89}$$

and

$$\partial_{\mu} \frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu} \psi_{x}\right)} = \frac{\partial \mathcal{L}}{\partial \psi_{x}} \Leftrightarrow i \partial_{\mu} \left(\bar{\psi}_{x} \gamma^{\mu}\right) + m \bar{\psi}_{x} = 0 \tag{10.90}$$

Is equation (10.89) the adjoint of (10.90)? Remember that to take the adjoint of a Dirac spinor we have to take the hermitean conjugate and then multiply by γ^5 , as in expression (10.82):

$$(-i)\partial_{\mu}\left(\psi_{x}^{\dagger}\gamma^{5}\gamma^{\mu}\right) + m\psi_{x}^{\dagger}\gamma^{5} = 0$$
(10.91)

Multiplying this equation on the right by γ^5 , and using $\gamma^5\gamma^5 = 1$ and

$$\left\{\gamma^5, \gamma^{\mu}\right\} = 0 \Rightarrow \gamma^5 \gamma^{\mu} \gamma^5 = -\gamma^{\mu} \tag{10.92}$$

we obtain the usual hermitean conjugate of the Dirac equation, $(-i\partial -m)\psi_x^{\dagger} = 0$. Having obtained the correct Lagrangian, we can now easily write down the action functional for the free Dirac field:

$$S = \int dx \; \bar{\psi}_x \left(i\gamma^\mu \partial_\mu - m \right) \psi \tag{10.93}$$

You clearly see that it is quadratic in the sense of the quadratic actions of Grassmann variables discussed in the first section of this chapter.

10.3.2 Dirac propagator

Comparing this action functional to the action functional of Grassmann variables in (10.25) we see that now

$$A_{xy} = (i\gamma^{\mu}\partial_{\mu} - m) \tag{10.94}$$

The Green's function $\tilde{G}(x-y)$ is its inverse,

$$(i\gamma^{\mu}\partial_{\mu} - m)\tilde{G}(x - y) = \delta(x - y).$$
(10.95)

We find it –as in the case of bosonic fields– by going to reciprocal space

$$\tilde{G}(k) = \int dr \; \tilde{G}(r) e^{ikr} \tag{10.96}$$

$$\tilde{G}(x-y) = \int \frac{dk}{(2\pi)^4} \tilde{G}(k) e^{-ik(x-y)}$$
(10.97)

we get

$$(k - m)\tilde{G}(k) = 1$$
 (10.98)

$$\Leftrightarrow \quad \tilde{G}(k) = \frac{1}{\not{k} - m} = \frac{\not{k} + m}{k^2 - m^2} \tag{10.99}$$

Keep in mind that $\hat{G}(k)$ is a 4×4 matrix, as can be seen most clearly from the last equality. If you work out k in the Weyl representation, you find

$$\tilde{G}(k) = \frac{1}{k^2 - m^2} \begin{pmatrix} m & 0 & k_0 + k_3 & k_1 - ik_2 \\ 0 & m & k_1 + ik_2 & k_0 - k_3 \\ \hline k_0 - k_3 & -k_1 + ik_2 & m & 0 \\ -k_1 - ik_2 & k_0 + k_3 & 0 & m \end{pmatrix}$$
(10.100)

Note moreover that $(\not k + m)(\not k - m)$ is equal to the unit matrix times $k^2 - m^2$.

The reason I put a tilde in $\tilde{G}(k)$ is because this is not the final form that I want to use. I will add $+i\varepsilon$ to the denominator, just as we did for the bosons:

$$G(k) = \frac{1}{\not k - m + i\varepsilon} = \frac{\not k + m}{k^2 - m^2 + i\varepsilon}.$$
 (10.101)

This is no longer to assure convergence of the integral – but to get the right time ordering in the fermion pair expectation value. Indeed, if we look at the pair expectation value, we could choose which order of the Grassmann variables we use! Going back to our general formulas (10.29) tot (10.32), we see that

$$\tilde{G}(x-y) = -i \left\langle \psi_x \bar{\psi}_y \right\rangle \tag{10.102}$$

The $+i\varepsilon$ factor assures that the real-space Green's function is related to the pair expectation value through

$$G(x-y) = -i \left\langle \psi_x \bar{\psi}_y \right\rangle \Theta(x_0 > y_0) + i \left\langle \bar{\psi}_y \psi_x \right\rangle \Theta(x_0 < y_0)$$
(10.103)

This means that we put the Grassmann variable with the earliest time (in the lab frame) to the right, and keep *chronological ordering*. Any re-ordering that corresponds to an odd permutation gets a minus sign... and these minus signs will also render Wick's decomposition rule more complicated. We can rewrite G(x - y) as

$$G(x-y) = \tilde{G}(x-y)\Theta(x_0 > y_0) - \tilde{G}(y-x)\Theta(x_0 < y_0)$$
(10.104)

Another way to rewrite G(x - y) is to use the time-ordering operator \mathcal{T} ,

$$G(x-y) = -i \left\langle \mathcal{T} \left[\psi_x \bar{\psi}_y \right] \right\rangle \tag{10.105}$$

where, the action of operator is to order the variables chronologically, with the earliest time to the right.

REMARK – In order to see that the $+i\varepsilon$ prescription is compatibe with (10.105), we calculate G(x - y) with from G(k) through the inverse Fourier transform. Notations: $(x - y)^{\mu} = (t, \vec{r}), k^{\mu} = (\omega, \vec{k})$. With $E_{\vec{k}} = \sqrt{\vec{k}^2 + m^2}$ we associate the on-shell $K^{\mu} = (E_{\vec{k}}, \vec{k})$ In these notations:

$$G(x-y) = \int \frac{d\omega}{2\pi} \int \frac{d\vec{k}}{(2\pi)^3} G(k) e^{-i\omega t} e^{+i\vec{k}\vec{r}}$$
$$= \int \frac{d\vec{k}}{(2\pi)^3} e^{+i\vec{k}\vec{r}} \int \frac{d\omega}{2\pi} \frac{\not{k}+m}{\omega^2 - \vec{k}^2 - m^2 + i\varepsilon} e^{-i\omega t} \quad (10.106)$$

The integral over ω can be performed with contour integration over a large half-circle. The poles of the integrand are located at $\omega = \pm \sqrt{\vec{k}^2 + m^2 - i\varepsilon} = \pm E_{\vec{k}} \mp i\varepsilon$ with ε still a positive infinitesimal. Hence

$$G(x-y) = \int \frac{d\vec{k}}{(2\pi)^3} e^{+i\vec{k}\vec{r}} \left(\vec{k}+m\right) \int \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\left(\omega-E_{\vec{k}}+i\varepsilon\right)\left(\omega+E_{\vec{k}}-i\varepsilon\right)}$$
(10.107)

When t > 0, we are forced to close (counterclockwise) along the lower half plane, containing the pole at $z = E_{\vec{k}} - i\varepsilon$. When t < 0 we are forced to close (clockwise) over the upper half plane, enclosing the pole at $z = -E_{\vec{k}} + i\varepsilon$. This is the reason why the result is split up between the different time orderings. Different ordering choices² can be obtained by shifting the poles to different sides of the real axis. We get (dropping ε as it has played its role):

$$G(x-y) = \int \frac{d\vec{k}}{(2\pi)^3} e^{+i\vec{k}\vec{r}} (\not{k}+m) \left(i\frac{e^{-iE_kt}}{2E_{\vec{k}}}\Theta(t>0) -i\frac{e^{+iE_kt}}{-2E_{\vec{k}}}\Theta(t>0)\right)$$
(10.108)

In the t < 0 part we can integrate over $-\vec{k}$ rather than \vec{k} , and obtain

The \vec{k} integrations are precisely the Fourier integrations of $\tilde{G}(k)$ after doing the k^0 integrations (swapping also the spinoral indices), so that $G(x - y) = \tilde{G}(x - y)\Theta(x_0 > y_0) - \tilde{G}(y - x)\Theta(x_0 < y_0)$ is satisfied.

The real-spacetime propagator looks complicated, but luckily we work with Feynman diagrams in reciprocal space and all we'll need is (10.101). This is

²In particular, the advanced Green's function $G^{>}(x-y) = -i \langle \psi_x \bar{\psi}_y \rangle \Theta(x^0 > y^0)$ and the retarded Green's function $G^{<}(x-y) = +i \langle \bar{\psi}_y \psi_x \rangle \Theta(x^0 < y^0)$ will pop up often in the literature. They are the separate pieces of our G(x-y).

more good news: in actual calculations of scattering cross sections and selfenergies you can very often get by without thinking of the fact that you work with Grassmann variables, and you may also worry less about the nasty time ordering stuff.

10.3.3 Including local U(1) gauge symmetry

Local U(1) gauge symmetry states that we can replace the Dirac spinors by $\psi(x) \rightarrow \psi(x)e^{i\theta(x)}$ with $\theta(r)$ a local phase, and this will leave the action invariant. We have seen how to do this in the part on classical field theory: we have to replace the partial derivatives with covariant derivatives

$$\partial_{\mu} \to D_{\mu} = \partial_{\mu} + iqA_{\mu} \tag{10.110}$$

Here -q is just a proportionality constant that we factored out of the gauge field A_{μ} This does alter the gauge invariance, and when you write out the field equations you find that it is just the electrical charge of the Fermi field. Hence, our first step is to write

$$\mathcal{L}(\psi, \partial_{\mu}\psi) = \bar{\psi} (i\gamma^{\mu}D_{\mu} - m)\psi$$

= $\bar{\psi} (i\not\!\!D - m)\psi$ (10.111)

We have again used Feynman's slash notation for $\not{D} = \gamma^{\mu} D_{\mu}$. This is of course not the full result – we have only written down the part of the Lagrangian concerning the Dirac field, we still need to include the parts $\mathcal{L}(A_{\mu}, \partial_{\nu} A_{\mu})$. Also this is something that we studied before, and found it to be

$$\mathcal{L}(A_{\mu}, \partial_{\nu} A_{\mu}) = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$
(10.112)

with $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$. Hence, the complete Lagrangian of a Dirac field together with a U(1) gauge field is

$$\mathcal{L}(\psi,\partial_{\mu}\psi,A_{\mu},\partial_{\nu}A_{\mu}) = \bar{\psi}\left(i\not\!\!D - m\right)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}$$
(10.113)

This can be written out to emphasise the interaction part between the gauge field and the Dirac field:

$$\mathcal{L}_{QED} = \underbrace{\bar{\psi}\left(i\partial \!\!\!/ - m\right)\psi}_{\text{free fermion}} \underbrace{-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}}_{\text{free photon}} \underbrace{-q\bar{\psi}A\psi}_{\text{interaction}}$$
(10.114)

with of course $A = \gamma^{\mu} A_{\mu}$. This is the famous Lagrangian of quantum electrodynamics, or QED. This was the first true quantum field theory that was developed. Just for fun, let's check whether it really is gauge invariant. The gauge transformation is

$$\psi \rightarrow \psi e^{i\theta(x)}$$
(10.115)

$$\bar{\psi} \rightarrow \bar{\psi}e^{-i\theta(x)}$$
 (10.116)

$$A_{\mu} \rightarrow A_{\mu} - \frac{1}{q} \partial_{\mu} \theta$$
 (10.117)

The last line corresponds to 6.30 with the extra factor -q that we introduced here just because it provided us with something we can link to the historical interpretation of electrical charge. The term $m\bar{\psi}\psi$ is obviously invariant. Also

$$\partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu} \to \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu} - \frac{1}{q}\left(\partial_{\mu}\partial_{\nu}\theta - \partial_{\nu}\partial_{\mu}\theta\right)$$
(10.118)

is invariant since the terms between brackets cancel. The remaining part is a bit more difficult:

$$\bar{\psi}\gamma^{\mu} \left[\partial_{\mu} + iqA_{\mu}\right]\psi \rightarrow \left(\bar{\psi}e^{-i\theta(x)}\right)\gamma^{\mu} \left[\partial_{\mu} + iq\left(A_{\mu} - \frac{1}{q}\partial_{\mu}\theta\right)\right]\left(\psi e^{i\theta(x)}\right) \\
= \bar{\psi}\gamma^{\mu} \left[\partial_{\mu}\psi + \psi i\partial_{\mu}\theta\right]$$
(10.119)

Now we use

$$\partial_{\mu}\left(\psi e^{i\theta(x)}\right) = e^{i\theta(x)}\left(\partial_{\mu}\psi + \psi i\partial_{\mu}\theta\right)$$

to obtain

$$\begin{split} \bar{\psi}\gamma^{\mu}\left[\partial_{\mu}+iqA_{\mu}\right]\psi &\to \bar{\psi}\gamma^{\mu}\left[\partial_{\mu}\psi+\psi i\left(\partial_{\mu}\theta\right)+iq\left(A_{\mu}-\frac{1}{q}\left(\partial_{\mu}\theta\right)\right)\psi\right]\\ &= \bar{\psi}\gamma^{\mu}\left[\partial_{\mu}+iqA_{\mu}\right]\psi+i\bar{\psi}\gamma^{\mu}\psi\left[\left(\partial_{\mu}\theta\right)-\frac{1}{q}q\left(\partial_{\mu}\theta\right)\right] \end{split}$$

And since the last terms again cancel, we have indeed shown local gauge invariance. Finally, let's see what the Noether current for this invariance would correspond to? Remember that the Noether current is given by

$$J^{\mu} = \frac{\partial \mathcal{L}}{\partial (\partial_{\mu}\psi)} \delta \psi + \frac{\partial \mathcal{L}}{\partial (\partial_{\mu}\bar{\psi})} \delta \bar{\psi}$$
(10.120)

The changes in the fields for an infinitesimal gauge transform are $\psi \to \psi e^{i\varepsilon} \approx \psi + i\psi\varepsilon$ so $\delta\psi = i\psi$. Similarly $\delta\bar{\psi} = i\bar{\psi}$. Now,

$$\frac{\partial \mathcal{L}}{\partial \left(\partial_{\mu} \bar{\psi}\right)} = 0 \tag{10.121}$$

$$\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \psi)} = i \bar{\psi} \gamma^{\mu} \qquad (10.122)$$

Hence $J^{\mu} = -\bar{\psi}\gamma^{\mu}\psi$. To go from this "field current" to a "charge current" (i.e. to introduce our electrical units of charge), we define the electrical current as

$$J^{\mu} = -q\bar{\psi}\gamma^{\mu}\psi \tag{10.123}$$

Hence, we can also write the QED Lagrangian as

$$\mathcal{L}_{QED} = \bar{\psi} \left(i \partial \!\!\!/ - m \right) \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + J^{\mu} A_{\mu} \tag{10.124}$$

The Noether current related to the Dirac field is the source term for the electromagnetic field. Charges and currents are indeed the sources of electrical and magnetic fields. We got this impressive structure – the theory of the electromagnetism of matter – in essence by imposing symmetry requirements on our model. Lorentz invariance and parity leads us to the Dirac field, and demanding in addition also local U(1) gauge invariance brings in all of electromagnetism.

Part IV

Application to many-body physics

Chapter 11

Fields at non-zero temperatures

Up till now, we have studied vacuum-to-vacuum transition amplitudes, but when the system is coupled to a bath at a certain temperature, the state with respect to which we want to calculate expectation values is no longer the vacuum, but the quantum-statistical equilibrium state. We need to use statistical mechanics, and make ensemble averages to predict the outcome of experiments. This is particularly important when applying field theory to many-body systems where we have many more degrees of freedom than the thermodynamic variables that we are interested in (free energy, specific heat, magnetization,... of the system).

11.1 Statistical mechanics and path integrals

11.1.1 Quantum statistical physics

Before tackling the problem of hot *fields*, we take a step back and review how *statistical mechanics* and *quantum mechanics* come together. The logic of statistical physics follows four easy steps:

- Step 1: The universe is divided up in the system we want to study and the rest of the world. The system is usually small in comparison to the rest of the world, so that this rest can be treated as a reservoir that is relatively insensitive to the changes in the system under scrutiny.
- Step 2: The (so-called "pure") quantum state of the system is a vector in a Hilbert space, for which we can choose a basis, preferably the energy-eigenkets $|\varphi_n\rangle$ (here quantum mechanics differs from classical mechanics where the state space does not have the structure of a vector space).
- Step 3: The rest of the world is seen as a reservoir interacting with the subsystem that we study, and as a result the quantum state of this system

is fluctuating, and entangled with the state of the reservoir. By tracing out the rest of the world we loose information (in particular the information about the state of the system), and we have to introduce a probability distribution telling us the probability for the system to be in one or other pure state. In particular, for systems in which energy is conserved, we set up a probability distribution p_n to find the system in energy eigenket $|\varphi_n\rangle$.

• Step 4: The fundamental assumption of statistical physics tells us something about this probability distribution, namely: in thermodynamic equilibrium, all states with the same energy are equally probable. That is why the energy eigenkets $|\varphi_n\rangle$ are a good choice for a basis. The probability associated with $|\varphi_n\rangle$ having energy E_n , is then $p_n = \exp\{-E_n/(k_BT)\}$ where T is the temperature (and k_B the Boltzmann constant).

These conceptual steps lead us to the well-known formula for the *partition sum* (the normalization of the probability distribution p_n),

$$\mathcal{Z} = \sum_{n} e^{-E_n/(k_B T)} \tag{11.1}$$

The unnormalized probability distribution is the *density matrix*:

$$\hat{\rho} = e^{-\hat{H}/(k_B T)} \tag{11.2}$$

We can write this in the basis of the energy eigenstates by taking a spectral decomposition:

$$\hat{\rho} = \sum_{n} e^{-E_n/(k_B T)} |\varphi_n\rangle \langle\varphi_n|$$
(11.3)

The density matrix gives access to the partition sum \mathcal{Z} by taking the trace,

$$\mathcal{Z} = \operatorname{Tr}\left[\hat{\rho}\right] = \int dx \, \left\langle x \left| \hat{\rho} \right| x \right\rangle, \qquad (11.4)$$

where

$$\langle x | \hat{\rho} | x \rangle = \left\langle x \left| e^{-\hat{H}/(k_B T)} \right| x \right\rangle.$$
 (11.5)

Substituting the spectal decomposition in this expectation value yields

$$\mathcal{Z} = \sum_{n} e^{-E_n/(k_B T)} \int dx \ \varphi_n^*(x) \varphi_n(x). \tag{11.6}$$

Since the eigenfunctions of the Hamiltonian are orthonormal, this indeed gives us the same result as (11.1). We want to calculate the thermodynamics of fields, and for this the partition sum is the central quantity to calculate. It is linked to the free energy F(T, V) by $\mathcal{Z} = e^{-F/(k_B T)}$ so that

$$F = -k_B T \log(\mathcal{Z}) = -k_B T \log\left[\operatorname{Tr}\left(\hat{\rho}\right)\right].$$
(11.7)

The density matrix is also useful to calculate quantum statistical expectation values of operators: these are found by tracing the operators over $\hat{\rho}$ as follows:

$$\left\langle \left\langle \hat{A} \right\rangle \right\rangle = \frac{1}{\mathcal{Z}} \operatorname{Tr} \left[\hat{\rho} \hat{A} \right].$$
 (11.8)

The double angular brackets emphasize that we average not only over the wavefunction (quantum fluctuations also present for a pure state) but also over the ensemble (classical statistical fluctuations).

11.1.2 Partition sum as a path integral

To see how this is linked to path integrals, consider the amplitude for a particle to be in position q_a at time t_a , and arrive in position q_b at time t_b . This amplitude is given by is

$$\left\langle q_b \left| e^{-i\hat{H}(t_b - t_a)/\hbar} \right| q_a \right\rangle.$$
 (11.9)

We start in the quantum state $|q_a\rangle$, apply the time evolution operator $e^{i\hat{H}(t_b-t_a)/\hbar}$ to let it evolve from time t_a to a final time t_b , and the project the result back onto $|q_b\rangle$ to find the aforementioned amplitude. From our discussion of path integrals in the first chapter on quantizing fields, we know that this same amplitude can also be written as a sum over all paths q(t) from (q_a, t_a) to (q_b, t_b) , weighed by $\exp\{iS[q(t)]/\hbar\}$:

$$\left\langle q_b \left| e^{-i\hat{H}(t_b - t_a)/\hbar} \right| q_a \right\rangle = \int \mathcal{D}q \, \exp\left\{ \frac{i}{\hbar} S[q] \right\},$$
 (11.10)

with S the action functional, for example for a usual Lagrangian

$$\left\langle q_b \left| e^{-i\hat{H}(t_b - t_a)/\hbar} \right| q_a \right\rangle = \int\limits_{(q_a, t_a)}^{(q_b, t_b)} \mathcal{D}q \exp\left\{ \frac{i}{\hbar} \int\limits_{t_a}^{t_b} \left[\frac{m}{2} \dot{q}^2 - V(q) \right] dt \right\}$$
(11.11)

Now, notice the similarity between (11.5) and (11.9): upon equating

$$\frac{i}{\hbar} \left(t_b - t_a \right) \leftrightarrow \frac{1}{k_B T} \tag{11.12}$$

you get the same formula. Thus, the density matrix can be obtained as a quantum mechanical transition amplitude obtained by evolving a ket along the *imaginary time* axis.

Let's see what this becomes in practice. We want a change of variables from t to τ , given by

$$\tau = i\left(t - t_a\right),\tag{11.13}$$

Hence

$$t = t_a \to \tau = 0 \tag{11.14}$$

$$t = t_b \to \tau = i(t_b - t_a) = \hbar\beta \tag{11.15}$$

with $\beta = 1/(k_B T)$ the inverse temperature. Thus, in the left hand side of (11.11) we get

$$\left\langle q_b \left| e^{-i\hat{H}(t_b - t_a)/\hbar} \right| q_a \right\rangle \longrightarrow \left\langle q_b \left| e^{-\beta\hat{H}} \right| q_a \right\rangle$$
 (11.16)

Furthermore, $dt = -id\tau$, and

$$\frac{dq}{dt} = \frac{dq}{d\tau}\frac{d\tau}{dt} = i\frac{dq}{d\tau} \Rightarrow \left(\frac{dq}{dt}\right)^2 = -\left(\frac{dq}{d\tau}\right)^2$$

so that $iS[q(t)]/\hbar$ transforms to

$$\frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[\frac{m}{2} \left(\frac{dq}{dt} \right)^2 - V(q) \right] = \frac{i}{\hbar} (-i) \int_{0}^{\hbar\beta} d\tau \left[-\frac{m}{2} \left(\frac{dq}{d\tau} \right)^2 - V(q) \right] 11.17)$$
$$= -\frac{1}{\hbar} \int_{0}^{\hbar\beta} d\tau \left[\frac{m}{2} \left(\frac{dq}{d\tau} \right)^2 + V(q) \right]_{S_E[q(\tau)]}$$
(11.18)

The underlined part is known as the *Euclidean action functional*, differing in some signs from the usual action functional. Putting all this together, expression (11.11) becomes

$$\left\langle q_b \left| e^{-\beta \hat{H}} \right| q_a \right\rangle = \int_{(q_a,0)}^{(q_b,\hbar\beta)} \mathcal{D}q \exp\left\{ -\frac{1}{\hbar} S_E \left[q(\tau) \right] \right\}$$
(11.19)

Here, the path integral can again be understood through (imaginary) time slicing. Divide the interval $[0, \hbar\beta]$ in steps $\delta\tau = \hbar\beta/N$, set $q_j = q(j\delta\tau)$ and sum over all possible paths by replacing

$$\int_{(q_a,0)}^{(q_b,\hbar\beta)} \mathcal{D}q \longrightarrow \int dq_0 \int dq_1 \dots \int dq_{N-1} \int dq_N \ \delta(q_0 = q_a) \delta(q_N = q_b) \quad (11.20)$$

Finally, take the limit for N very large. Note that the weights are now true (real-valued) Gaussians, and not interfering (complex) phase factors! This type of (very well-behaved) path integral has been well studied in mathematics, where it is known as a *Wiener path integral*, named after Norbert Wiener.

11.2. EUCLIDEAN QUANTUM FIELD THEORY

To obtain the partition sum through (11.4), we have to set $q_b = q_a$, and integrate over q_a . Thus, we find the main result for the quantum statistical mechanics of a single quantum particle:

$$\mathcal{Z} = \int_{q(0)=q(\hbar\beta)} \mathcal{D}q \exp\left\{-\frac{1}{\hbar}S_E\left[q(\tau)\right]\right\},\tag{11.21}$$

with

$$\int_{q(0)=q(\hbar\beta)} \longrightarrow \int dq_0 \int dq_1 \dots \int dq_{N-1} \int dq_N \ \delta(q_0 = q_N). \tag{11.22}$$

Basically, this is a review of what some of you may have seen already in our course on path integration. Here, we need to extend this idea from one particle to many particles, and to a field, just as we did for propagation in real time when we quantized classical fields.

11.2 Euclidean quantum field theory

Moving from particles to fields, we go from integrals of Lagrangian over time to integrals over Lagrangian densities over spacetime. When we switch now from real time to imaginary time, we get

$$d^4x = dt d\vec{x} \to -i d\tau d\vec{x} = -i d_E^4 x \tag{11.23}$$

Now it is also clear where the name "Euclidean" comes from:

$$-d_E^4 x = -(id\tau)^2 + (dx)^2 + (dy)^2 + (dz)^2$$

= $(d\tau)^2 + (dx)^2 + (dy)^2 + (dz)^2$ (11.24)

we get a Euclidean flat space, even with a simple Cartesian metric. Recall our example of a springy string. Adding a mass term and some interaction potential, we had

$$\mathcal{L} = \frac{1}{2} \partial^{\mu} \varphi \partial_{\mu} \varphi - \frac{m^2}{2} \varphi^2 - V(\varphi).$$
 (11.25)

The kinetic energy part changes,

$$\partial^{\mu}\varphi\partial_{\mu}\varphi = \left(\partial_{t}\varphi\right)^{2} - \left(\partial_{\vec{x}}\varphi\right)^{2} \longrightarrow - \left(\partial_{\tau}\varphi\right)^{2} - \left(\partial_{\vec{x}}\varphi\right)^{2}, \qquad (11.26)$$

so that

$$\mathcal{L} \to -\frac{1}{2} \left[\left(\partial_\tau \varphi \right)^2 + \left(\partial_{\vec{x}} \varphi \right)^2 + m^2 \varphi^2 \right] - V(\varphi).$$
 (11.27)

The phase factor $\exp\{iS[\varphi]\}$ (recall that for quantum field theory we had set $\hbar = 1$) changes to

$$\exp\left\{iS[\varphi]\right\} = \exp\left\{i\int d^4x \left[\frac{1}{2}\partial^{\mu}\varphi\partial_{\mu}\varphi - \frac{m^2}{2}\varphi^2 - V(\varphi)\right]\right\}$$
$$\rightarrow \exp\left\{-\int d^4_E x \left[\frac{1}{2}\left(\partial_{\tau}\varphi\right)^2 + \frac{1}{2}\left(\partial_{\vec{x}}\varphi\right)^2 + \frac{m^2}{2}\varphi^2 + V(\varphi)\right]\right\}$$

we can write this as $\exp\{-S_E[\varphi]\}$ with (after partial integration)

$$S_E[\varphi] = \int_0^\beta d\tau \int d\vec{x} \left[\frac{1}{2} \varphi \left(-\partial_\tau^2 - \nabla_{\vec{x}}^2 + m^2 \right) \varphi + V(\varphi) \right]$$
(11.29)

the Euclidean field action (for a real, bosonic field).

The partition sum of the field can then be found in analogy to the prescription for single particles, through

$$\mathcal{Z}_B = \int_{\varphi(\vec{x},0)=\varphi(\vec{x},\beta)} \mathcal{D}\varphi \exp\left\{-S_E\left[\varphi\right]\right\}.$$
 (11.30)

Once again, we can interpret the integral over all possible field configurations by going to the discretized spacetime picture, and integrating over all the field values at all spacetime points. Now, there is an additional restriction that the final and initial spatial configurations are the same. The subscript B in the partition sum tells us that his is a partition sum of a *Bosonic field*. For a fermionic field, a pesky minus sign appears in the boundary:

$$\mathcal{Z}_F = \int_{\psi(\vec{x},0) = -\psi(\vec{x},\hbar\beta)} \mathcal{D}\psi \exp\left\{-S_E\left[\psi\right]\right\},\tag{11.31}$$

due to the properties of the Grassmann variables. Quantum statistical expectation values, of some functionals $F[\varphi]$ of the field, are then computed as

$$\langle\langle F \rangle\rangle = \frac{1}{\mathcal{Z}_B} \int_{\substack{\varphi(\vec{x},0) = \varphi(\vec{x},\beta)}} \mathcal{D}\varphi \ F[\varphi] \exp\left\{-S_E[\varphi]\right\}$$
(11.32)

These results are central to this chapter, and can be summarized following A. Zee as:

Euclidean quantum field theory in (D+1)-dimensional spacetime with $\tau \in [0, \beta]$ is equivalent to Quantum statistical mechanics in *D*dimensional space at a temperature $k_B T = 1/\beta$ (where boundary conditions tell you if you deal with bosons or fermions).
11.3 Free field free energy

11.3.1 The trace-log formula

In our previous chapters on quantum field theory, we were actually preparing for the Euclidean quantum field theory by not always including the "i" explicitly. We found that for quadratic actions of (complex) bosonic fields the functional integral reduces to

$$\exp\left\{-\sum_{x,y}\phi_x^*A_{xy}\phi_y\right\}\longrightarrow \mathcal{Z}_B = \frac{1}{\det(A)}.$$
(11.33)

For quadratic actions of fermionic (Grassmann) fields we similarly obtained

$$\exp\left\{-\sum_{x,y}\bar{\psi}_{x}A_{xy}\psi_{y}\right\}\longrightarrow\mathcal{Z}_{F}=\det\left(A\right)$$
(11.34)

For the Minkowskian quantum field theory, the one with the "i" in front of A_{xy} , we hand-wavingly carried the *i* through to the final formulas, noting that we may need some $i\varepsilon$ terms as convergence factors. So, now that we're investigating quantum statistical mechanics, our formulas are actually better behaved and we need less waving of hands. We can just use our results (11.33) and (11.34). Note that the determinant of a (symmetric or hermitean) matrix is equal to the product of the (real) eigenvalues λ_n ,

$$\det\left(A\right) = \prod_{n} \lambda_{n} \tag{11.35}$$

By taking the exponential of the logarithm of this we can rewrite the determinant as

$$\det(A) = \exp\left\{\log\left[\prod_{n} \lambda_{n}\right]\right\} = \exp\left\{\sum_{n} \log\left[\lambda_{n}\right]\right\}$$
(11.36)

The sum of the logarithms of the eigenvalues is actually just the trace of the logarithm of the matrix A (this follows from the definition of the logarithm of a matrix):

$$\det (A) = \exp \left\{ \operatorname{Tr} \left[\log \left(A \right) \right] \right\}. \tag{11.37}$$

This is the very useful "trace-log formula". It allows to rewrite the partition sums for bosons and fermions as

$$\mathcal{Z}_B = \exp\left\{-\operatorname{Tr}\left[\log\left(A\right)\right]\right\},\qquad(11.38)$$

$$\mathcal{Z}_F = \exp\left\{+\operatorname{Tr}\left[\log\left(A\right)\right]\right\}. \tag{11.39}$$

To evaluate this, we need to diagonalise A – a recurring theme in this course. In order to diagonalise something like

$$A \leftrightarrow \left(-\partial_{\tau}^2 - \nabla_{\vec{x}}^2 + m^2\right) \tag{11.40}$$

we went to reciprocal space. For the spatial piece nothing changes, and we can Fourier transform our fields from \vec{x} to \vec{k} dependence. However, in the time domain things are very different now: we have a finite domain $\tau \in [0, \hbar\beta]$ in which the fields are either periodic (bosons) or antiperiodic (fermions). Rather than doing Fourier transforms, we will require Fourier series.

11.3.2 Matsubara frequencies

We can decompose any function that is periodic in $\tau \in [0, \beta]$ (i.e. any function which satisfies $\phi(0) = \phi(\beta)$) in Fourier components with frequency $\omega_n = 2\pi n/\beta$. Since this periodicity condition holds for bosonic fields, the frequencies are called

Bosonic Matsubara frequencies:
$$\omega_n = 2n\pi/\beta$$
. (11.41)

For fermions, the functions are antiperiodic, i.e. $\psi(0) = -\psi(\beta)$. Such functions can be decomposed in Fourier components with odd frequencies $(2n+1)\pi/\beta$. These are called

Fermionic Matsubara frequencies:
$$\omega_n = (2n+1)\pi/\beta.$$
 (11.42)

Using these notations, the imaginary time domain can be represented in a unified notation as the Fourier series

$$f(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \tilde{f}(i\omega_n) e^{-i\omega_n \tau}$$
(11.43)

$$\tilde{f}(i\omega_n) = \int_0^\beta d\tau \ f(\tau)e^{+i\omega_n\tau}$$
(11.44)

Substituting these into each other, we find the representations for the delta function and for the Kronecker delta:

$$\delta(\tau - \tau') = \frac{1}{\beta} \sum_{n = -\infty}^{\infty} \exp\left\{\pm i\omega_n \left(\tau - \tau'\right)\right\}$$
(11.45)

$$\delta_{n,n'} = \int_0^\beta d\tau \, \exp\left\{\pm i \left(\omega_n - \omega_{n'}\right)\tau\right\}$$
(11.46)

where both signs give the same result.

Now we want to combine the Fourier transform to wave numbers with the Fourier series in Matsubara frequencies to transform the fields (bosonic, grass-mann, sources,...) as follows:

$$\phi(\vec{k},n) = \int_0^\beta d\tau \int d\vec{x} \,\phi(\vec{x},\tau) \exp\left\{i\omega_n\tau - i\vec{k}\cdot\vec{x}\right\}$$
(11.47)

$$\phi(\vec{x},\tau) = \frac{1}{\beta} \sum_{n} \int \frac{d\vec{k}}{(2\pi)^3} \phi(\vec{k},n) \exp\left\{-i\omega_n\tau + i\vec{k}\cdot\vec{x}\right\}$$
(11.48)

11.3. FREE FIELD FREE ENERGY

Different sign conventions are possible, you just have to choose one and stick to it. We've chosen one that reminds us of the spacetime to reciprocal space transform that we used before. Now we're ready to transform the Euclidean action functional (and I keep using a complex bosonic field as the example):

$$S_E[\phi] = \int_0^\beta d\tau \int d\vec{x} \ \phi^*(\vec{x},\tau) \left[-\partial_\tau^2 - \nabla_{\vec{x}}^2 + m^2 \right] \phi(\vec{x},\tau).$$
(11.49)

Substitute the Fourier decompositions for ϕ and for its complex conjugate ϕ^* to obtain

$$S_E[\phi] = \int_0^\beta d\tau \int d\vec{x} \left(\frac{1}{\beta} \sum_{n'} \int \frac{d\vec{k}'}{(2\pi)^3} \phi^*(\vec{k}', n') e^{i\omega_{n'}\tau - i\vec{k}' \cdot \vec{x}} \right) \\ \times \left[-\partial_\tau^2 - \nabla_{\vec{x}}^2 + m^2 \right] \left(\frac{1}{\beta} \sum_n \int \frac{d\vec{k}}{(2\pi)^3} \phi(\vec{k}, n) e^{-i\omega_n\tau + i\vec{k} \cdot \vec{x}} \right)$$
(1.50)

The derivatives now only work on the exponential

$$\left[-\partial_{\tau}^{2} - \nabla_{\vec{x}}^{2} + m^{2}\right] e^{-i\omega_{n}\tau + i\vec{k}\cdot\vec{x}} = e^{-i\omega_{n}\tau + i\vec{k}\cdot\vec{x}} \left[\omega_{n}^{2} + \vec{k}^{2} + m^{2}\right]$$
(11.51)

and collect all the remaining pieces with τ and \vec{x} :

$$S_{E}[\phi] = \frac{1}{\beta} \sum_{n'} \int \frac{d\vec{k'}}{(2\pi)^{3}} \frac{1}{\beta} \sum_{n} \int \frac{d\vec{k}}{(2\pi)^{3}} \phi^{*}(\vec{k'}, n') \left[\omega_{n}^{2} + \vec{k'}^{2} + m^{2}\right] \phi(\vec{k}, n)$$

$$\times \underbrace{\int_{0}^{\beta} d\tau \exp\left\{i\left(\omega_{n'} - \omega_{n}\right)\tau\right\}}_{\beta\delta_{n,n'}} \underbrace{\int d\vec{x} \exp\left\{i\left(\vec{k} - \vec{k'}\right) \cdot \vec{x}\right\}}_{(2\pi)^{3}\delta(\vec{k} - \vec{k'})}$$
(11.52)

The delta's allow to get rid of the primed variables,

$$S_E[\phi] = \frac{1}{\beta} \sum_n \int \frac{d\vec{k}}{(2\pi)^3} \phi^*(\vec{k}', n') \left[\omega_n^2 + \vec{k}^2 + m^2\right] \phi(\vec{k}, n)$$
(11.53)

Hence, in reciprocal space A is diagonal!

$$A_{\vec{k},n;\vec{k}',n'} = \left[\omega_n^2 + \vec{k}^2 + m^2\right]\delta_{n,n'}\delta(\vec{k} - \vec{k}')$$
(11.54)

The logarithms of a diagonal matrix is found by taking the logarithm of its diagonal elements:

$$\log(A)_{\vec{k},n;\vec{k}',n'} = \log\left[\omega_n^2 + \vec{k}^2 + m^2\right]\delta_{n,n'}\delta(\vec{k} - \vec{k}')$$
(11.55)

Taking the trace of this means summing over all diagonal elements, i.e. summing over all n (n' = n) and integrating over all \vec{k} (with $\vec{k}' = \vec{k}$, and) with a density of states in k-space of V/ $(2\pi)^3$ where V is the volume of the system:

Tr
$$[\log(A)] = \frac{V}{(2\pi)^3} \int d\vec{k} \sum_{n=-\infty}^{\infty} \log\left[\omega_n^2 + \vec{k}^2 + m^2\right]$$
 (11.56)

Now we can use the trace-log formula to obtain

$$\mathcal{Z}_B = \exp\left\{-\frac{\mathrm{V}}{(2\pi)^3} \int d\vec{k} \sum_{n=-\infty}^{\infty} \log\left[\omega_n^2 + \vec{k}^2 + m^2\right]\right\}$$
(11.57)

In fact, we could just as well have done this with Grassmann fields, and get the same S_E just by writing ψ 's in stead of ϕ 's. This would give

$$\mathcal{Z}_F = \exp\left\{ +\frac{\mathrm{V}}{(2\pi)^3} \int d\vec{k} \sum_{n=-\infty}^{\infty} \log\left[\omega_n^2 + \vec{k}^2 + m^2\right] \right\}$$
(11.58)

The free energy can be extracted from the partition sum as $F = -k_B T \log(\mathcal{Z})$, so that for bosons

$$F_B = +\frac{\mathrm{V}}{(2\pi)^3\beta} \int d\vec{k} \sum_{n=-\infty}^{\infty} \log\left[\left(\omega_n^{bose}\right)^2 + \vec{k}^2 + m^2\right]$$
(11.59)

with $\omega_n^{bose} = 2n\pi/\beta$, and for fermions

$$F_F = -\frac{\mathrm{V}}{(2\pi)^3\beta} \int d\vec{k} \sum_{n=-\infty}^{\infty} \log\left[\left(\omega_n^{fermi}\right)^2 + \vec{k}^2 + m^2\right]$$
(11.60)

with $\omega_n^{fermi} = (2n+1)\pi/\beta$. This starts to resemble a formula that we know from statistical mechanics for the free energy of a free Bose gas or a free Fermi gas as an integral over \vec{k} space. However, there are still these nasty Matsubara summations to take. To do that, we need a wee bit of complex analysis. As I told you at the onset of this course, all you previous theoretical physics and maths-for-physicist courses come together in this QFT...

11.4 Matsubara summations

11.4.1 Summing series with contour integrals

The residue theorem from complex analysis allows you to rewrite a summation as a contour integral. For simple summation, the basic formula looks as follows

$$\sum_{n=m}^{p} f(n) = \frac{1}{2\pi i} \oint_{C} \pi f(z) \cot(\pi z) dz - \sum_{\substack{\text{poles of } f(z) \\ \text{in the contour}}} \operatorname{Res} \left[\pi f(z) \cot(\pi z)\right] (11.61)$$

Here we have assumed that

- f(z) is a meromorphic function (it only has isolated points as poles), and
- that the poles of f(z) and of $\cot(\pi z)$ do not coincide, and



Figure 11.1: Cotangent in the complex plane

• that the contour C encompasses the poles of $\cot(\pi z)$ for z = m, ..., p.

Why does the cotangent $\cot(\pi z) = \cos(\pi z)/\sin(\pi z)$ appear in this formula? The cotangens turns out tohave poles of first order wherever $\sin(\pi z)$ becomes zero, i.e. wherever $z = n \in \mathbb{Z}$. The residues in these poles are

$$\operatorname{Res}_{z=n} \left[\pi f(z) \operatorname{cotg}(\pi z) \right] = \lim_{z \to n} \left[\pi f(z) \operatorname{cotg}(\pi z)(z-n) \right].$$
(11.62)

Here $(z - n) / \sin(\pi z)$ has a removable singularity in z = n:

$$\lim_{z \to n} \left[\frac{(z-n)}{\sin(\pi z)} \right] = \frac{(-1)^n}{\pi}.$$
 (11.63)

So, the residues of the integrand in (11.61) are

$$\operatorname{Res}_{z=n} \left[\pi f(z) \operatorname{cotg}(\pi z) \right] = \frac{(-1)^n}{\pi} \pi f(n) \cos(\pi n) = f(n)$$
(11.64)

The residue theorum plucks just the values of the function f(z) in the points z = n out of the area enclosed by the contour. That is why we introduce the cotangent. Figure 11.1 shows the amplitude and phase of the cotangent in the complex plane (the phase is represented by a color, going from red (phase 0) over the rainbow to violet and back to red. The zeroes and poles along the real axis are clearly visible. Wandering away from the real axis into the complex plane the cotangent goes to one.

If we take a contour that contains the poles z = m, ..., p then we have taken into account the function values f(m), ..., f(p). Of course we could still have



Figure 11.2: The Bose-Einstein distribution $1/(e^{\beta z} - 1)$ in the complex plane.

walked around poles of f(z) itself, so we obtain

$$\frac{1}{2\pi i} \oint_C \pi f(z) \cot(\pi z) dz = \sum_{n=m}^p f(n) + \sum_{\substack{\text{poles of } f(z)\\\text{in the contour}}} \operatorname{Res}\left[\pi f(z) \cot(\pi z)\right],$$
(11.65)

from which our first formula follows. This formula illustrates the general principle: multiply the function f(z) that you need to sum with another function that picks out the values of f(z) that you need in the summation. So, let's apply this to summations over Matsubara frequencies.

11.4.2 Enter Bose and Fermi distributions

In quantum statistical calculations with fields, we will often have to make Matsubara summations, that we can write as

$$\frac{1}{\beta} \sum_{n=-\infty}^{\infty} f(i\omega_n) \tag{11.66}$$

We want to transform these sums into integrals, as we did with (11.61). So, we need to multiply the analytic continuation of the function f(z) with a function that picks out precisely the values $f(i\omega_n)$ with ω_n the bosonic or fermionic Matsubara frequencies. This must be a function which has poles in $z = i\omega_n =$ $i(2n\pi/\beta)$ for bosons, and poles in $z = i\omega_n = i(2n+1)\pi/\beta$ for fermions.

Let's first look at the case of bosons. We want to have a function with poles along the imaginary axis at $i(2n\pi/\beta)$, and nowhere else (also not in infinity!). This strong restriction fixes the function (up to a multiplicative constant).



Figure 11.3: The Fermi-Dirac distribution $1/(e^{\beta z} + 1)$ in the complex plane.

Now comes impressive magic, in the meeting of complex analysis and quantum statistics: it turns out that this function is the Bose-Einstein distribution

$$n_B(z) = \frac{1}{e^{\beta z} - 1}.$$
(11.67)

How this function looks in the complex plane is shown in figure 11.2. Again, the height shows the amplitude, and the colors show the phase (red=0, over the rainbow to light blue= π and via indigo back to red=also 2π). The function remains finite everywhere except in to points $2\pi i n/\beta$. There it clearly has poles, and from the figure we can see that these are poles of first order – since, as you walk around the pole, the colors go through the color circle once. The residue at a pole $z = i\omega_n^{bose}$ is given by

$$\operatorname{Res}_{z=2n\pi/\beta} \left[\frac{1}{e^{\beta z} - 1} \right] = \lim_{z \to 2n\pi/\beta} \frac{z - 2n\pi/\beta}{e^{\beta z} - 1}$$
(11.68)

We can find this limit with l'Hôpital's rule:

$$\lim_{z \to 2n\pi/\beta} \frac{z - i2n\pi/\beta}{e^{\beta z} - 1} = \lim_{z \to 2n\pi/\beta} \frac{1}{\beta e^{\beta z}} = \frac{1}{\beta e^{2n\pi}} = \frac{1}{\beta}$$
(11.69)

Note that when z lies on the real axis, the function $n_B(z)$ turns back to the usual Bose-Einstein distribution. How nice that bosonic Matsubara frequencies link through the complex plane with the Bose-Einstein distribution.

For the case of fermions you can already guess that we'll need the function

$$n_F(z) = \frac{1}{e^{\beta z} + 1} \tag{11.70}$$

This will link the fermionic Matsubara frequencies firmly to the Fermi-Dirac distribution. Indeed, the function $n_F(z)$ has poles precisely in $z = i(2n+1)\pi/\beta$,



Figure 11.4: A contour for doing the Matsubara summation.

as you can see in figure 11.3. As before, height shows the amplitude (modulus) and color indicates the phase of this complex function. Again we have first order poles, and their residues are

$$\operatorname{Res}_{z=(2n+1)\pi/\beta} \left[\frac{1}{e^{\beta z} + 1} \right] = \lim_{z \to (2n+1)\pi/\beta} \frac{z - i(2n+1)\pi/\beta}{e^{\beta z} + 1} \quad (11.71)$$

$$= \lim_{z \to (2n+1)\pi/\beta} \frac{z}{\beta e^{\beta z}} = -\frac{1}{\beta}$$
(11.72)

which follows from l'Hôpital's rule as in the bosonic case.

11.4.3 Matsubara contour integrals

Now we can use the auxiliary functions $n_B(z)$ and $n_F(z)$ to rewrite bosonic and fermionic Matsubara summations $\frac{1}{\beta} \sum_n f(i\omega_n)$ as contour integrals. We have to use a contour that will contain all the poles of the auxiliary function, for example a large circle as shown in figure 11.4.The contour integral is equal to the sum of the residues of all the poles inside it. Assuming that f(z) has no poles that coincide with $n_{B,F}(z)$, we get the following contribution from the poles at Matsubara frequencies ω_n . If we start with the fermionic case, these poles contribute already the following residues:

$$\operatorname{Res}_{z=i\omega_n} \left[\frac{f(z)}{e^{\beta z} + 1} \right] = \lim_{z \to i\omega_n} \left[\frac{f(z)}{e^{\beta z} + 1} (z - i\omega_n) \right]$$
(11.73)

Note that if f(z) turns out to have poles $z = i\omega_n$ this is still no disaster, but then you have to treat that one pole separately. If it doesn't, then we can replace f(z) by $f(i\omega_n)$ and obtain

$$\operatorname{Res}_{z=i\omega_n} \left[\frac{f(z)}{e^{\beta z} + 1} \right] = f(i\omega_n) \lim_{z \to i\omega_n} \left(\frac{z - i\omega_n}{e^{\beta z} + 1} \right) = -\frac{f(i\omega_n)}{\beta}$$
(11.74)

11.5. HOT FERMIONS

Adding to this the contributions from poles of f(z) itself, we get

$$\frac{1}{2\pi i} \oint_C f(z) n_F(z) = -\frac{1}{\beta} \sum_{n=-\infty}^{\infty} f(i\omega_n) + \sum_{\text{polen } z_j \text{ van } f} \operatorname{Res}_{z=z_j} \left[f(z) n_F(z) \right] \quad (11.75)$$

The function $n_F(z)$ has done her work well: we obtain the Matsubara sum that we want. Now, if we have in addition that $f(z)n_F(z)$ goes to zero for $|z| \to \infty$ faster than $|z|^{-1}$, the contribution from the large circle will vanish – we find

Fermi:
$$\frac{1}{\beta} \sum_{n=-\infty}^{\infty} f(i\omega_n) = \sum_{\text{poles } z_j \text{ of } f} \operatorname{Res}_{z=z_j} [f(z)n_F(z)].$$
 (11.76)

We find an analogous formula for the sum over bosonic Matsubara frequencies by replacing n_F by n_B ; and we obtain a sign change because of the signs of the residues. The formula becomes

Bose:
$$\frac{1}{\beta} \sum_{n=-\infty}^{\infty} f(i\omega_n) = -\sum_{\text{poles } z_j \text{ of } f} \operatorname{Res}_{z=z_j} [f(z)n_B(z)]$$
(11.77)

You may think that the contribution of the large circle always vanishes, since you have an exponential in the denominator. But look at figures 11.2 and 11.3: in the complex plane these functions (modulus square) go to one in the left half plane – they only go exponentially to zero in the right half plane. Hence, you need to check that the function f(z) goes to zero fast enough in the left half plane. And sometimes other horror stories appear: branch points and branch cuts. Actually, for our example of a free bosonic or free fermionic field, this is exactly what happens: from formulas (11.59),(11.60) for the free energy it is seen that we want to evaluate matsubara sums of the form

$$\mathcal{I} = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \ln\left[\omega_n^2 + \vec{k}^2 + m^2\right]$$

$$= \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \left[\ln\left(i\omega_n + \sqrt{\vec{k}^2 + m^2}\right) + \ln\left(-i\omega_n + \sqrt{\vec{k}^2 + m^2}\right)\right]$$
(11.78)

Hence we'll have

$$f(z) = \ln\left(z \pm \sqrt{\vec{k}^2 + m^2}\right) \tag{11.79}$$

to investigate... This logarithm has a branch point at $z = \mp E_{\vec{k}}$, with as usual $E_{\vec{k}} = \sqrt{\vec{k}^2 + m^2}$.

11.5 Hot fermions

Let's solve a useful example, and calculate the fermionic Matsubara sum

$$\mathcal{I} = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \ln\left(i\omega_n - E\right)$$
(11.80)



Figure 11.5: Amplitude and phase of $n_F(z) \ln(z-E) e^{-\epsilon z}$.

To perform this summation, we need to consider the analytic continuation

$$f(z) = e^{-\epsilon z} \operatorname{Ln} \left(z - E \right) \tag{11.81}$$

We take the main branch of the logarithm, $\operatorname{Ln}(re^{i\theta}) = \ln(r) + i\theta$, and indicate this by the capital letter L in logarithm. Furthermore, ϵ is an infinitesimal positive number, a convergence factor,

$$\mathcal{I} = \lim_{\epsilon \to 0} \left[\frac{1}{\beta} \sum_{n = -\infty}^{\infty} f(i\omega_n) \right].$$
(11.82)

If you use a large circle with radius going to infinity, there are a few difficulties to tackle:

- 1. Does the function $f(z)n_F(z)$ go to zero faster than $|z|^{-1}$ when |z| goes to infinity? This is why we need the convergence factor $e^{-\epsilon\tau}$. The combination $\ln(z-E)n_F(z)$ goes to zero for $\operatorname{Re}[z] \to +\infty$ but diverges for $\operatorname{Re}[z] \to -\infty$. The additional factor $e^{-\epsilon\tau}$ keeps the integrand wellbehaved, as can be seen from figure 11.5where the modulus and phase of the integrand are shown. This means the large circle will not contribute to the contour integral: its contribution will vanish as its radius R goes to zero.
- 2. The function f(z) has a branch cut, starting in the branch point z = E. We can put the branch cut along the positive real axis. Contours can't cross branch cuts, so we have to walk around it via two straight lines Γ_1 and Γ_2 , and a small circle C_{δ} , as indicated in figure 11.6. The small circle will not contribute to the integral, since $\delta \ln(\delta)$ goes to zero for $\delta \to 0$.



Figure 11.6: Contour chosen for the Matsubara summation.

So, the contour integral consists of four pieces: the large circle C_R , de lines Γ_1 and Γ_2 , and the small circle C_{δ} :

$$\oint f(z)n_F(z)dz = \int_{C_R} f(z)n_F(z)dz + \int_{R-i\varepsilon}^{E-i\varepsilon} f(x)n_F(x)dx + \int_{C_\delta} f(z)n_F(z)dz + \int_{E+i\varepsilon}^{R+i\varepsilon} f(x)n_F(x)dx, \quad (11.83)$$

of which two pieces vanish. The two remaining pieces give

$$\oint f(z)n_F(z)dz = \int_E^R f(x+i\varepsilon)n_F(x+i\varepsilon)dx - \int_E^R f(x-i\varepsilon)n_F(x-i\varepsilon)dx \quad (11.84)$$

The Fermi function is continuous across the real axis, so that for ε infinitesimal

$$n_F(x+i\varepsilon)e^{-\epsilon(x+i\varepsilon)} = n_F(x-i\varepsilon)e^{-\epsilon(x-i\varepsilon)} = n_F(x)e^{-\epsilon x}.$$
 (11.85)

Hence we obtain

$$\oint f(z)n_F(z)dz = \int_E^R \left[\operatorname{Ln}(x+i\varepsilon) - \operatorname{Ln}(x-i\varepsilon)\right] n_F(x)e^{-\epsilon x}dx.$$
(11.86)

The logarithm jumps by $2\pi i$ as we cross the branch cut, so that

$$Ln(x + i\varepsilon) - Ln(x - i\varepsilon) = [Ln(x) + i0] - [Ln(x) + i2\pi] = -2\pi i.$$
(11.87)

The result for the contour integral then becomes

$$\oint f(z)n_F(z)dz = -2\pi i \int_E^R n_F(x)e^{-\epsilon x}dx \qquad (11.88)$$

This must be equal to the sum of residues of poles contained within the contour. These poles are precisely the fermionic Matsubara frequencies, resulting in

$$\frac{1}{2\pi i} \oint f(z) n_F(z) dz = -\frac{1}{\beta} \sum_{n=-\infty}^{\infty} f(i\omega_n)$$
(11.89)

Taking the limits $R \to \infty$ and $\epsilon \to 0_+$ we find the result for our Matsubara summation

$$\frac{1}{\beta} \sum_{n=-\infty}^{\infty} f(i\omega_n) = \int_{E}^{\infty} n_F(x) dx$$
(11.90)

All we need to do is the integral over the Fermi-Dirac distribution:

$$\frac{1}{\beta}\sum_{n=-\infty}^{\infty}f(i\omega_n) = \int_E^{\infty}\frac{1}{e^{\beta x}+1}dx = \int_E^{\infty}\frac{e^{-\beta x}}{1+e^{-\beta x}}dx$$
(11.91)

This can be done by writing it as a power series, or simply by a change of integration variable to $u = e^{-\beta x}$:

$$\int_{E}^{\infty} \frac{e^{-\beta x}}{1 + e^{-\beta x}} dx = \frac{1}{\beta} \int_{0}^{e^{-\beta E}} \frac{1}{1 + u} du = \frac{1}{\beta} \operatorname{Ln} \left(1 + e^{-\beta E} \right)$$
(11.92)

Thus, we get as a result for this Matsubara summation:

$$\sum_{n=-\infty}^{\infty} \operatorname{Ln}\left(i\omega_n - E\right) = \operatorname{Ln}\left(1 + e^{-\beta E}\right).$$
(11.93)

Going back to the free energy for the Fermi gas, expression (11.60), we see that

$$F_F = -\frac{\mathrm{V}}{(2\pi)^3\beta} \int d\vec{k} \sum_{n=-\infty}^{\infty} \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \left[\ln\left(i\omega_n - E_{\vec{k}}\right) + \ln\left(-i\omega_n - E_{\vec{k}}\right) \right]$$
(11.94)

We get a positive and a negative energy solution (as we know happens in the relativistic case). Focusing on the positive energy solution, we get

$$F_F = -\frac{V}{(2\pi)^3\beta} \int d\vec{k} \ln\left(1 + e^{-\beta E_{\vec{k}}}\right)$$

$$\Rightarrow F_F = -\sum_{\vec{k}} k_B T \ln\left(1 + e^{-\beta E_{\vec{k}}}\right). \qquad (11.95)$$

This is exactly the formula that you have seen in the introductory course on statistical mechanics! Similarly, for the Bose gas we get

$$F_B = +\sum_{\vec{k}} k_B T \ln \left(1 - e^{-\beta E_{\vec{k}}} \right).$$
(11.96)

which also follows from the bosonic Matsubara summation.

Chapter 12

The BEC-BCS transition

In this chapter we look at a very specific application, namely pairing and superfluidity of a system of interacting fermionic atoms. This will illustrate how we set up a field theory to describe a system, how we tackle interactions (in a way different from simple perturbation theory) and how we investigate the free energy of this system to figure out a phase diagram. It is moreover an example very relevant to the research community on ultracold atoms.

12.1 Ultracold atomic Fermi gases

In the study of superconductivity, ultracold quantum gases offer a singular advantage over condensed matter systems in that their system parameters can be tuned experimentally with a high degree of precision and over a wide range. For example, the interaction strength between fermionic atoms is tunable by an external magnetic field. This field can be used to vary the scattering length over a Feshbach resonance, from a large negative to a large positive value. In the limit of large negative scatting lengths, a cloud of ultracold fermionic atoms will undergo cooper pairing, and exhibit superfluidity when cooled below the critical temperature. On the other side of the resonance, at large positive scattering lengths, a molecular bound state gets admixed to the scattering state, and a Bose-Einstein condensate (BEC) of fermionic dimers can form. With the magnetically tunable s-wave scattering length, the entire crossover region between the Bardeen-Cooper-Schrieffer (BCS) superfluid and the molecular BEC can be investigated in a way that is thus far not possible in solids.

Also the amount of atoms in each hyperfine state can be tuned experimentally with high precision. Typically, fermionic atoms (such as 40 K or 6 Li) are trapped in two different hyperfine states. These two hyperfine spin states provide the "spin-up" and "spin-down" partners that form the Cooper pairs. Unlike in metals, in quantum gases the individual amounts of "spin-up" and "spindown" components of the Fermi gas can be set independently (using evaporative cooling and Rabi oscillations). This allows to investigate how Cooper pairing (and the ensuing superfluidity) is frustrated when there is no equal amount of spin ups and spin downs, i.e. in the so-called "(spin-)imbalanced Fermi gas". In a superconducting metal, the magnetic field that would be required to provide a substantial imbalance between spin-up and spin-down electrons is simply expelled by the Meissner effect, so that the imbalanced situation cannot be studied. The particular question of the effect of spin-imbalance is of great current interest¹, and we will keep our treatment general enough to include this effect.

Finally, the geometry of the gas is adaptable. Counterpropagating laser beams can be used to make periodic potentials for the atoms, called "optical lattices". Imposing such a lattice in just one direction transforms the atomic cloud into a stack of pancake-shaped clouds, with tunable tunneling amplitude between pancakes. The confinement in the out-of-pancake direction can be made tight enough to allow to study the physics of the two-dimensional system effectively. Imposing an optical lattice in more than one direction, all manner of crystals can be formed, and it becomes possible to engineer an experimental realization of the Bose and Fermi Hubbard models, for example. The joint tunability of number of atoms, temperature, dimensionality, interaction strength has in the past couple of decades turned the quantum gases into powerful quantum simulators of condensed matter models². In this respect, ultracold quantum gases are also being used to enlarge our knowledge of superconductivity, through the study of pairing and superfluidity.

A key aspect of ultracold quantum gases is that the interatomic interaction can be characterized by a single number, the s-wave scattering length mentioned above. In fact, the requirement to use the label "ultracold" is that the typical wave lengths associated with the atomic motion is much larger than the range of the interatomic potential, so that higher partial waves in the scattering process are frozen out. This aspect allows to simplify the treatment of the interatomic interactions tremendously. Rather than using a complicated interatomic potential, we can use a contact pseudopotential $V(\mathbf{r} - \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}')$, and adapt its strength g such that the model- or pseudopotential has the same s-wave scattering length as the true potential. Doing so requires some care³, and using the Lippmann-Schwinger equation up to second order results in the following expression for the renormalized strength g of the contact interaction (in the three dimensional case):

$$\frac{1}{g} = \frac{m}{4\pi\hbar^2 a_s} - \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{\hbar^2 k^2/m}.$$
(12.1)

Moreover, for a Fermi-gas there is an additional simplification: due to the obligation of antisymmetrizing the wave function the s-wave scattering amplitude

¹A book gathering a lot of information and reports of recent research in ultracold Fermi gases is: M. Inguscio, W. Ketterle, and C. Salomon, *Ultra-cold Fermi gases* (IOS press, Amsterdam, the Netherlands, 2007).

²A review can be found in: I. Bloch, J. Dalibard, and W. Zwerger, *Many-body physics with ultracold gases*, Rev. Mod. Phys. **80**, 885 (2008).

³Check out these books for more information: C.J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge UK, 2008), and H.T.C. Stoof, K.B. Gubbels, and D.B.M. Dickerscheid, *Ultracold Quantum Fields* (Springer, 2009).

between fermions with the same (hyperfine) spin is zero. This means that in an ultracold Fermi gas, only atoms with different spin states interact. This allows us to write the action functional for the Fermi gas of atoms with mass m as

$$\mathcal{S}\left[\left\{\bar{\psi}_{\mathbf{x},\tau,\sigma},\psi_{\mathbf{x},\tau,\sigma}\right\}\right] = \int_{0}^{\hbar\beta} d\tau \int d\mathbf{x} \sum_{\sigma} \left[\bar{\psi}_{\mathbf{x},\tau,\sigma} \left(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla_{\mathbf{x}}^2 - \mu_{\sigma}\right)\psi_{\mathbf{x},\tau,\sigma}\right] \\ + \int_{0}^{\hbar\beta} d\tau \int d\mathbf{x} \int d\mathbf{y} \;\bar{\psi}_{\mathbf{x},\tau,\uparrow}\bar{\psi}_{\mathbf{y},\tau,\downarrow} \; g\delta(\mathbf{x}-\mathbf{y}) \;\psi_{\mathbf{y},\tau,\downarrow}\psi_{\mathbf{x},\tau,\uparrow}.$$
(12.2)

Here, $\beta = 1/(k_B T)$ is again the inverse temperature. The quadratic term corresponds to the free particle Lagrangian. The amounts of spin up $\sigma = \uparrow$ and spin down $\sigma = \downarrow$ are set by the chemical potentials μ_{\uparrow} and μ_{\downarrow} , respectively. It is the total particle density $n_{\uparrow} + n_{\downarrow}$ that is used to define a Fermi wave vector: $k_F = (3\pi^2(n_{\uparrow} + n_{\downarrow}))^{1/3}$ in three dimensions, and $k_F = (2\pi(n_{\uparrow} + n_{\downarrow}))^{1/2}$ in two dimensions. The quartic term corresponds to the interaction part, and we have used the contact pseudopotential.

To keep our notations simple and make integrals and variables dimensionless, we will introduce natural units of k_F , the Fermi wave number, and E_F , the Fermi energy. Also we use $\omega_F = E_F/\hbar$ for frequency unit and $T_F = E_F/k_B$ for temperature unit [so this all comes down to setting $\hbar, 2m, k_F, k_B = 1$]. Note that since the fields have units of volume^{-1/2}, the action has units of \hbar . Moreover, ghas units of energy times volume, since $g\delta(\mathbf{x} - \mathbf{y})$ is a potential energy. Change to the dimensionless space/time variables $\mathbf{x}' = \mathbf{x}k_F$ and $\tau' = E_F \tau/\hbar$, we get

$$\mathcal{S}\left[\left\{\psi_{\mathbf{x},\tau,\sigma},\psi_{\mathbf{x},\tau,\sigma}\right\}\right] = \int_{0}^{T_{F}/T} \frac{\hbar d\tau'}{E_{F}} \int d\mathbf{x}' \sum_{\sigma} \left[\bar{\psi}_{\mathbf{x}',\tau',\sigma} \left(E_{F} \frac{\partial}{\partial\tau'} - \frac{\hbar^{2}k_{F}^{2}}{2m} \nabla_{\mathbf{x}'}^{2} - \mu_{\sigma}\right) \psi_{\mathbf{x}',\tau',\sigma}\right] \quad (12.3) + \int_{0}^{T_{F}/T} \frac{\hbar d\tau'}{E_{F}} \int d\mathbf{x}' \int d\mathbf{y}' \ \bar{\psi}_{\mathbf{x}',\tau',\uparrow} \bar{\psi}_{\mathbf{y}',\tau',\downarrow} \ g\left[k_{F}^{3}\delta(\mathbf{x}'-\mathbf{y}')\right] \ \psi_{\mathbf{y}',\tau',\downarrow} \psi_{\mathbf{x}',\tau',\uparrow}.$$

$$(12.4)$$

Since $\bar{\psi}_{\mathbf{x},\tau,\sigma}\psi_{\mathbf{x},\tau,\sigma}d\mathbf{x}$ was dimensionless to start with, it must be equal to the corresponding expression with the primed variables. Introducing $\mu'_{\sigma} = \mu_{\sigma}/E_F$,

 $\beta' = \beta E_F$ and $g' = gk_F^3/E_F$, and using that $E_F = (\hbar k_F)^2/(2m)$ we get

$$\mathcal{S}\left[\left\{\bar{\psi}_{\mathbf{x},\tau,\sigma},\psi_{\mathbf{x},\tau,\sigma}\right\}\right] = \hbar \int_{0}^{\beta'} d\tau' \int d\mathbf{x}' \sum_{\sigma} \left[\bar{\psi}_{\mathbf{x}',\tau',\sigma} \left(\frac{\partial}{\partial\tau'} - \boldsymbol{\nabla}_{\mathbf{x}'}^{2} - \mu_{\sigma}'\right)\psi_{\mathbf{x}',\tau',\sigma}\right] \\ + \hbar g' \int_{0}^{\beta'} d\tau' \int d\mathbf{x}' \ \bar{\psi}_{\mathbf{x}',\tau',\uparrow} \bar{\psi}_{\mathbf{x}',\tau',\downarrow} \psi_{\mathbf{x}',\tau',\downarrow} \psi_{\mathbf{x}',\tau',\uparrow}.$$
(12.5)

Finally, note that, in our units (with $\mathbf{k}' = \mathbf{k}/k_F$) the renormalized strength of the contact potential is

$$\frac{1}{g'} = \frac{1}{8\pi k_F a_s} - \int \frac{d\mathbf{k}'}{(2\pi)^3} \frac{1}{2(k')^2}.$$
(12.6)

Dropping the primes, we get the starting point of our treatment:

$$\mathcal{Z} = \int \mathcal{D}\psi \exp\left\{-\int_{0}^{\beta} d\tau \int d\mathbf{x} \sum_{\sigma} \bar{\psi}_{\mathbf{x},\tau,\sigma} \left(\frac{\partial}{\partial \tau} - \boldsymbol{\nabla}_{\mathbf{x}}^{2} - \mu_{\sigma}\right) \psi_{\mathbf{x},\tau,\sigma} -g \int_{0}^{\beta} d\tau \int d\mathbf{x} \ \bar{\psi}_{\mathbf{x},\tau,\uparrow} \bar{\psi}_{\mathbf{x},\tau,\downarrow} \psi_{\mathbf{x},\tau,\downarrow} \psi_{\mathbf{x},\tau,\uparrow} \right\}.$$
(12.7)

This is, if you will, the statement of the problem that we want to investigate. Working with the operator version of quantum mechanics, you would state your starting Hamiltonian – in the path integral formalism, you have to state your starting action functional. Ours describes a gas of fermionic particles, of two spin species (with the possibility of spin imbalance), with contact interactions between particles of different spins. The goal of our calculation is to obtain the free energy of the system (so that we have access to its thermodynamics), and to identify the superfluid phase (and its order parameter). This is done in five main steps, and in the following subsections we go through them in detail.



Figure 12.1: Illustration of the Hubbard-Stratonovic transformation: the interaction term originally comprised of a product of four fermion fields is decomposed in a term that represents two fermions pairing up, a term for the propagation of the pairs (not shown) and a term for the pair breaking up into two fermions.

12.2 Hubbard-Stratonovic fields

12.2.1 The Hubbard-Stratonovic transformation

The Hubbard-Stratonovic transformation is based on the Gaussian integral formula for completing the squares:

$$\exp\left\{-g\int_{0}^{\beta}d\tau\int d\mathbf{x}\;\bar{\psi}_{\mathbf{x},\tau,\uparrow}\bar{\psi}_{\mathbf{x},\tau,\downarrow}\psi_{\mathbf{x},\tau,\downarrow}\psi_{\mathbf{x},\tau,\uparrow}\right\} = \int \mathcal{D}\Delta$$
$$\exp\left\{\int_{0}^{\beta}d\tau\int d\mathbf{x}\;\left[\frac{\bar{\Delta}_{\mathbf{x},\tau}\Delta_{\mathbf{x},\tau}}{g} + \bar{\Delta}_{\mathbf{x},\tau}\psi_{\mathbf{x},\tau,\downarrow}\psi_{\mathbf{x},\tau,\uparrow} + \Delta_{\mathbf{x},\tau}\bar{\psi}_{\mathbf{x},\tau,\uparrow}\bar{\psi}_{\mathbf{x},\tau,\downarrow}\right]\right\}.$$
(12.8)

In this formula, the auxiliary fields $\bar{\Delta}_{\mathbf{x},\tau}$, $\Delta_{\mathbf{x},\tau}$ do not have a spin index and are complex *bosonic* fields and not Grassmann variables. We interpret this bosonic field as the field of the fermion pairs, as illustrated in figure (12.1). Using this in our starting point, expression (12.7), we get

$$\mathcal{Z} = \int \mathcal{D}\psi \int \mathcal{D}\Delta \exp\left\{-\int_{0}^{\beta} d\tau \int d\mathbf{x} \left[\sum_{\sigma} \bar{\psi}_{\mathbf{x},\tau,\sigma} \left(\frac{\partial}{\partial \tau} - \boldsymbol{\nabla}_{\mathbf{x}}^{2} - \mu_{\sigma}\right) \psi_{\mathbf{x},\tau,\sigma} + -\frac{\bar{\Delta}_{\mathbf{x},\tau} \Delta_{\mathbf{x},\tau}}{g} - \bar{\Delta}_{\mathbf{x},\tau} \psi_{\mathbf{x},\tau,\downarrow} \psi_{\mathbf{x},\tau,\uparrow} - \Delta_{\mathbf{x},\tau} \bar{\psi}_{\mathbf{x},\tau,\uparrow} \bar{\psi}_{\mathbf{x},\tau,\downarrow}\right]\right\}.$$
(12.9)

The resulting action is quadratic in the fermion fields, and can be integrated out easily when we introduce Nambu notation.

12.2.2 Nambu spinors

This combines a spin-up and a spin-down Fermi field into a new spinor, the Nambu spinor, given by

$$\eta_{\mathbf{x},\tau} = \begin{pmatrix} \psi_{\mathbf{x},\tau,\uparrow} \\ \bar{\psi}_{\mathbf{x},\tau,\downarrow} \end{pmatrix} \text{ and } \bar{\eta}_{\mathbf{x},\tau} = \begin{pmatrix} \bar{\psi}_{\mathbf{x},\tau,\uparrow} & \psi_{\mathbf{x},\tau,\downarrow} \end{pmatrix}, \qquad (12.10)$$

or, in component form

$$\begin{cases} \eta_{\mathbf{x},\tau,1} = \psi_{\mathbf{x},\tau,\uparrow} & \\ \eta_{\mathbf{x},\tau,2} = \bar{\psi}_{\mathbf{x},\tau,\downarrow} & \\ \end{cases} \quad \text{and} \begin{cases} \bar{\eta}_{\mathbf{x},\tau,1} = \bar{\psi}_{\mathbf{x},\tau,\uparrow} & \\ \bar{\eta}_{\mathbf{x},\tau,2} = \psi_{\mathbf{x},\tau,\downarrow} & \\ \end{cases}$$

Note that we have to take care about the measure of integration! The Grassmann path integral means by definition

$$\int \mathcal{D}\bar{\psi}_{\mathbf{x},\tau,\sigma} \mathcal{D}\psi_{\mathbf{x},\tau,\sigma} := \prod_{\mathbf{x},\tau,\sigma} \left(\int d\bar{\psi}_{\mathbf{x},\tau,\sigma} \int d\psi_{\mathbf{x},\tau,\sigma} \right)$$
$$= \prod_{\mathbf{x},\tau} \left(\int d\bar{\psi}_{\mathbf{x},\tau,\uparrow} \int d\psi_{\mathbf{x},\tau,\uparrow} \int d\bar{\psi}_{\mathbf{x},\tau,\downarrow} \int d\psi_{\mathbf{x},\tau,\downarrow} \right).$$

The factors (between brackets) in this product can be swapped as long as we keep the two fields together: so if we keep $d\bar{\psi}_{\mathbf{x},\tau,\sigma}d\psi_{\mathbf{x},\tau,\sigma}$ pairs together, the order of the $\{\mathbf{x},\tau,\sigma\}$ does not matter. The Grassmann path integral over the η spinors means by definition

$$\int \mathcal{D}\bar{\eta}_{\mathbf{x},\tau} \mathcal{D}\eta_{\mathbf{x},\tau} := \prod_{\mathbf{x},\tau} \left(\int d\bar{\eta}_{\mathbf{x},\tau,1} \int d\eta_{\mathbf{x},\tau,1} \int d\bar{\eta}_{\mathbf{x},\tau,2} \int d\eta_{\mathbf{x},\tau,2} \right).$$

Now replace component by component, to get

$$\int \mathcal{D}\bar{\eta}_{\mathbf{x},\tau} \mathcal{D}\eta_{\mathbf{x},\tau} = \prod_{\mathbf{x},\tau} \left(\int d\bar{\psi}_{\mathbf{x},\tau,\uparrow} \int d\psi_{\mathbf{x},\tau,\uparrow} \int d\psi_{\mathbf{x},\tau,\downarrow} \int d\bar{\psi}_{\mathbf{x},\tau,\downarrow} \right)$$
$$= \prod_{\mathbf{x},\tau} \left(-\int d\bar{\psi}_{\mathbf{x},\tau,\uparrow} \int d\psi_{\mathbf{x},\tau,\uparrow} \int d\bar{\psi}_{\mathbf{x},\tau,\downarrow} \int d\psi_{\mathbf{x},\tau,\downarrow} \right).$$

There is, for every \mathbf{x}, τ , a minus sign when compared to the measure of $\mathcal{D}\bar{\psi}_{\mathbf{x},\tau,\sigma}\mathcal{D}\psi_{\mathbf{x},\tau,\sigma}$:

$$\int \mathcal{D}\bar{\psi}_{\mathbf{x},\tau,\sigma} \mathcal{D}\psi_{\mathbf{x},\tau,\sigma} \to \int \mathcal{D}\bar{\eta}_{\mathbf{x},\tau} \mathcal{D}\eta_{\mathbf{x},\tau} \left[\prod_{\mathbf{x},\tau} (-1)\right].$$

This is important when taking the integrals! Indeed, for the Gaussian integral with coefficients $\mathbb{A}_{\mathbf{x},\tau}$ (these are 2 × 2 matrices since our Nambu spinors have 2 components):

$$\begin{split} &\int \mathcal{D}\bar{\psi}_{\mathbf{x},\tau,\sigma} \mathcal{D}\psi_{\mathbf{x},\tau,\sigma} \exp\left\{-\sum_{\mathbf{x},\tau} \bar{\eta}_{\mathbf{x},\tau} \cdot \mathbb{A}_{\mathbf{x},\tau} \cdot \eta_{\mathbf{x},\tau}\right\} \\ &= \prod_{\mathbf{x},\tau} \int d\bar{\psi}_{\mathbf{x},\tau,\uparrow} \int d\psi_{\mathbf{x},\tau,\uparrow} \int d\bar{\psi}_{\mathbf{x},\tau,\downarrow} \int d\psi_{\mathbf{x},\tau,\downarrow} \exp\left\{-\bar{\eta}_{\mathbf{x},\tau} \cdot \mathbb{A}_{\mathbf{x},\tau} \cdot \eta_{\mathbf{x},\tau}\right\} \\ &= \prod_{\mathbf{x},\tau} (-1) \int d\bar{\eta}_{\mathbf{x},\tau,1} \int d\eta_{\mathbf{x},\tau,1} \int d\bar{\eta}_{\mathbf{x},\tau,2} \int d\eta_{\mathbf{x},\tau,2} \exp\left\{-\bar{\eta}_{\mathbf{x},\tau} \cdot \mathbb{A}_{\mathbf{x},\tau} \cdot \eta_{\mathbf{x},\tau}\right\} \\ &= \prod_{\mathbf{x},\tau} (-1) \det_{\sigma} \left(\mathbb{A}_{\mathbf{x},\tau}\right). \end{split}$$

Note that the determinant here is only the determinant over the 2×2 matrix between the Nambu spinors, it is the "spinor determinant", indicated by a σ subscript. By exponentiating the logarithm we can write this as

$$\prod_{\mathbf{x},\tau} (-1) \det_{\sigma} (\mathbb{A}_{\mathbf{x},\tau}) = \prod_{\mathbf{x},\tau} \exp \left\{ \ln \left[-\det_{\sigma} (\mathbb{A}_{\mathbf{x},\tau}) \right] \right\} = \exp \left\{ \sum_{\mathbf{x},\tau} \ln \left[-\det_{\sigma} (\mathbb{A}_{\mathbf{x},\tau}) \right] \right\},$$

where with the sum we mean the trace:

$$\sum_{\mathbf{x},\tau} \ln \left[-\det_{\sigma} \left(\mathbb{A}_{\mathbf{x},\tau} \right) \right] = \operatorname{Tr} \left\{ \ln \left[-\det_{\sigma} \left(\mathbb{A}_{\mathbf{x},\tau} \right) \right] \right\},$$
(12.11)

which really is nothing else but

$$\int \mathcal{D}\bar{\psi}_{\mathbf{x},\tau,\sigma} \mathcal{D}\psi_{\mathbf{x},\tau,\sigma} \exp\left\{-\sum_{\mathbf{x},\tau} \bar{\eta}_{\mathbf{x},\tau} \cdot \mathbb{A}_{\mathbf{x},\tau} \cdot \eta_{\mathbf{x},\tau}\right\} = \exp\left\{\sum_{\mathbf{x},\tau} \ln\left[-\det_{\sigma}\left(\mathbb{A}_{\mathbf{x},\tau}\right)\right]\right\}.$$
(12.12)

So, the swap in order gives the minus sign in front of the determinant. Indeed, sometimes the integration measure does matter.

12.3 Effective action for the pair field

Now we still have to figure out what the matrix between the Nambu spinors is before we can perform the integrations over the Grassmann fields in (12.9). For reasons that become clear in the light of Green's functions, we will not call this matrix \mathbb{A} , but instead we will call it $-\mathbb{G}^{-1}$. and prove that

$$-\mathbb{G}^{-1} = \begin{pmatrix} \frac{\partial}{\partial \tau} - \nabla_{\mathbf{x}}^2 - \mu_{\uparrow} & -\Delta_{\mathbf{x},\tau} \\ -\bar{\Delta}_{\mathbf{x},\tau} & \frac{\partial}{\partial \tau} + \nabla_{\mathbf{x}}^2 + \mu_{\downarrow} \end{pmatrix}.$$
 (12.13)

We do this by expanding as follows

$$\bar{\eta}_{\mathbf{x},\tau} \cdot (-\mathbb{G}^{-1}) \cdot \eta_{\mathbf{x},\tau}$$
(12.14)
= $\left(\begin{array}{cc} \bar{\psi}_{\mathbf{x},\tau,\uparrow} & \psi_{\mathbf{x},\tau,\downarrow} \end{array} \right) \cdot \left(\begin{array}{cc} \frac{\partial}{\partial \tau} - \nabla_{\mathbf{x}}^2 - \mu_{\uparrow} & -\Delta_{\mathbf{x},\tau} \\ -\bar{\Delta}_{\mathbf{x},\tau} & \frac{\partial}{\partial \tau} + \nabla_{\mathbf{x}}^2 + \mu_{\downarrow} \end{array} \right) \cdot \left(\begin{array}{c} \psi_{\mathbf{x},\tau,\uparrow} \\ \bar{\psi}_{\mathbf{x},\tau,\downarrow} \end{array} \right).$

This gives

$$\bar{\eta}_{\mathbf{x},\tau} \cdot \left(-\mathbb{G}^{-1}\right) \cdot \eta_{\mathbf{x},\tau} = \bar{\psi}_{\mathbf{x},\tau,\uparrow} \left(\frac{\partial}{\partial \tau} - \nabla_{\mathbf{x}}^{2} - \mu_{\uparrow}\right) \psi_{\mathbf{x},\tau,\uparrow} - \Delta_{\mathbf{x},\tau} \bar{\psi}_{\mathbf{x},\tau,\uparrow} \bar{\psi}_{\mathbf{x},\tau,\downarrow} - \bar{\Delta}_{\mathbf{x},\tau} \psi_{\mathbf{x},\tau,\downarrow} \psi_{\mathbf{x},\tau,\uparrow} + \psi_{\mathbf{x},\tau,\downarrow} \left(\frac{\partial}{\partial \tau} + \nabla_{\mathbf{x}}^{2} + \mu_{\downarrow}\right) \bar{\psi}_{\mathbf{x},\tau,\downarrow}.$$

$$(12.15)$$

The first three terms in (12.15) are exactly as in the action in (12.9). The last term is more difficult since it involves a derivative that is positioned between two Grassmann variables. We know that when two Grassmann variables are swapped, they get a minus sign. To see what we should do with derivatives, we have to jump a bit ahead of ourselves and do the Fourier transforms. Then we get rid of the operator character of the derivatives, and we can clearly see what how the rules are. Starting from (see next section):

$$\psi_{\mathbf{x},\tau,\sigma} = \frac{1}{\sqrt{\beta V}} \sum_{n} \sum_{\mathbf{k}} e^{-i\omega_n \tau + i\mathbf{k} \cdot \mathbf{x}} \psi_{\mathbf{k},n,\sigma}, \qquad (12.16)$$

$$\bar{\psi}_{\mathbf{x},\tau,\sigma} = \frac{1}{\sqrt{\beta V}} \sum_{n} \sum_{\mathbf{k}} e^{i\omega_n \tau - i\mathbf{k} \cdot \mathbf{x}} \bar{\psi}_{\mathbf{k},n,\sigma}, \qquad (12.17)$$

we know what the derivative will mean

$$\psi_{\mathbf{x},\tau,\sigma}\left(\frac{\partial}{\partial\tau}\right)\bar{\psi}_{\mathbf{x},\tau,\sigma}\rightarrow\psi_{\mathbf{k},n,\sigma}\left(i\omega_{n}\bar{\psi}_{\mathbf{k},n,\sigma}\right).$$

Now there is no trouble in swapping the Grassmann variables, this just results in a minus sign:

$$\psi_{\mathbf{k},n,\sigma}\left(i\omega_n\bar{\psi}_{\mathbf{k},n,\sigma}\right)=\bar{\psi}_{\mathbf{k},n,\sigma}\left(-i\omega_n\right)\psi_{\mathbf{k},n,\sigma}.$$

But now we see that this is just equal to

$$\bar{\psi}_{\mathbf{x},\tau,\sigma}\left(\frac{\partial}{\partial\tau}\right)\psi_{\mathbf{x},\tau,\sigma}\rightarrow\bar{\psi}_{\mathbf{k},n,\sigma}\left(-i\omega_{n}\psi_{\mathbf{k},n,\sigma}\right).$$

So the rule is: if there is an odd-degree derivative sandwiched between two conjugate Grassmann variables, and these are swapped, there is no sign change. For second derivatives, there is again a sign change, for third derivatives again no change,.... If we now apply this newly gained knowledge to the fourth term of (12.15) we arrive at

$$\begin{split} \psi_{\mathbf{x},\tau,\downarrow} &\frac{\partial}{\partial \tau} \bar{\psi}_{\mathbf{x},\tau,\downarrow} + \psi_{\mathbf{x},\tau,\downarrow} \left(\nabla_{\mathbf{x}}^{2} + \mu_{\downarrow} \right) \bar{\psi}_{\mathbf{x},\tau,\downarrow} \\ &= -\bar{\psi}_{\mathbf{x},\tau,\downarrow} \left(-\frac{\partial}{\partial \tau} \right) \psi_{\mathbf{x},\tau,\downarrow} - \bar{\psi}_{\mathbf{x},\tau,\downarrow} \left(\nabla_{\mathbf{x}}^{2} + \mu_{\downarrow} \right) \psi_{\mathbf{x},\tau,\downarrow} \\ &= \bar{\psi}_{\mathbf{x},\tau,\downarrow} \left(\frac{\partial}{\partial \tau} - \nabla_{\mathbf{x}}^{2} - \mu_{\downarrow} \right) \psi_{\mathbf{x},\tau,\downarrow}. \end{split}$$

Now we see that the fourth term is indeed also equal to the corresponding term in (12.9).

Note that in general, the inverse Green's matrix $-\mathbb{G}_{\mathbf{x},\tau}^{-1}$ is not diagonal in \mathbf{x}, τ (for interactions other than the delta function). We should treat $-\mathbb{G}^{-1}$ as an operator in e.g. position representation, and write

$$\left\langle \mathbf{x}', \tau' \left| -\mathbb{G}^{-1} \right| \mathbf{x}, \tau \right\rangle = \left\langle \mathbf{x}', \tau' \right| \mathbf{x}, \tau \right\rangle \begin{pmatrix} \frac{\partial}{\partial \tau} - \nabla_{\mathbf{x}}^{2} - \mu_{\uparrow} & -\Delta_{\mathbf{x}, \tau} \\ -\bar{\Delta}_{\mathbf{x}, \tau} & \frac{\partial}{\partial \tau} + \nabla_{\mathbf{x}}^{2} + \mu_{\downarrow} \end{pmatrix}.$$
(12.18)

The matrix gives the operator in position (and time) representation. If it were not diagonal there would be terms like $\bar{\eta}_{\mathbf{x}',\tau'} \langle \mathbf{x}', \tau' | - \mathbb{G}^{-1} | \mathbf{x}, \tau \rangle \eta_{\mathbf{x},\tau}$ in the Gaussian integral and we would need to first diagonalize the whole spacetime matrix. Luckily, we are using a contact potential! Note that when the system is not interacting, there will be no pairs, and we get in position representation

$$-\mathbb{G}_{0}^{-1} \to \left(\begin{array}{cc} \frac{\partial}{\partial \tau} - \nabla_{\mathbf{x}}^{2} - \mu_{\uparrow} & 0\\ 0 & \frac{\partial}{\partial \tau} + \nabla_{\mathbf{x}}^{2} + \mu_{\downarrow} \end{array}\right).$$
(12.19)

So, in

$$\mathcal{Z} = \int \mathcal{D}\bar{\Delta}_{\mathbf{x},\tau} \mathcal{D}\Delta_{\mathbf{x},\tau} \int \mathcal{D}\bar{\psi}_{\mathbf{x},\tau,\sigma} \mathcal{D}\psi_{\mathbf{x},\tau,\sigma}$$
(12.20)

$$\times \exp\left\{-\int_{0}^{\beta} d\tau \int d\mathbf{x} \left[-\frac{\bar{\Delta}_{\mathbf{x},\tau}\Delta_{\mathbf{x},\tau}}{g} + \bar{\eta}_{\mathbf{x},\tau} \cdot \left(-\mathbb{G}_{\mathbf{x},\tau}^{-1}\right) \cdot \eta_{\mathbf{x},\tau}\right]\right\}$$

we can use our earlier result, expression (12.12) to obtain

$$\mathcal{Z} = \int \mathcal{D}\bar{\Delta}_{\mathbf{x},\tau} \mathcal{D}\Delta_{\mathbf{x},\tau} \exp\left\{-\int_{0}^{\beta} d\tau \int d\mathbf{x} \left[-\frac{\bar{\Delta}_{\mathbf{x},\tau}\Delta_{\mathbf{x},\tau}}{g} - \ln\left[-\det_{\sigma}\left(-\mathbb{G}_{\mathbf{x},\tau}^{-1}\right)\right]\right]\right\}.$$
(12.21)

This result does not contain any approximation (apart from the choice of starting Lagrangian). But, $-\mathbb{G}^{-1}$ depends on $\Delta_{\mathbf{x},\tau}$ and contains a bunch of derivatives too, so we have no way to calculate the logarithm of that (remember that the determinant is here the spinor determinant over the 2×2 matrix but, as noted earlier, there is no problem with that). We will need to go to reciprocal space. Rather than using the spacetime coordinates \mathbf{x}, τ we work in the space of wave numbers \mathbf{k} and Matsubara frequencies $\omega_n = (2n + 1)\pi/\beta$ for fermions and $\overline{\omega}_n = 2n\pi/\beta$ for bosons (both with $n \in \mathbb{Z}$).

12.4 Intermezzo: The long road to reciprocal space

The goal of this section is to rewrite (12.21) in reciprocal space, so that we can trace over the wave numbers and (Matsubara) frequencies rather than positions and times. The starting point for fermions is

$$\langle \mathbf{x}, \tau | \mathbf{k}, n \rangle = \frac{\exp\left\{i\mathbf{k} \cdot \mathbf{x}\right\}}{\sqrt{V}} \frac{e^{-i\omega_n \tau}}{\sqrt{\beta}}.$$
 (12.22)

For bosons we replace $\omega_n = (2n+1)\pi/\beta$ by $\varpi_n = 2n\pi/\beta$. The available wave numbers are the same for bosons as for fermions, they are given by

 $\{k_x, k_y, k_z\} = (2\pi/L) \{n_x, n_y, n_z\}$ with $n_x, n_y, n_z \in \mathbb{Z}$. There are various valid choices for normalizing the plane waves, and that tends to lead to quite some confusion in the results found in the literature. That is why we will go through quite some detail here to follow the effects of the choice of normalization that we have made here. We basically want the reciprocal space kets to obey the completeness relation

$$\mathbb{I} = \sum_{\mathbf{k},n} |\mathbf{k},n\rangle \langle \mathbf{k},n|. \qquad (12.23)$$

The spacetime kets obey

$$\mathbb{I} = \int_{0}^{\beta} d\tau \int d\mathbf{x} \, |\mathbf{x}, \tau\rangle \, \langle \mathbf{x}, \tau| \,.$$
(12.24)

This leads to the orthonormality relations

$$\langle \mathbf{k}, n | \mathbf{k}', n' \rangle = \delta(\mathbf{k} - \mathbf{k}') \delta_{nn'}. \tag{12.25}$$

The consistency of these relations can be proven by inserting expression (12.24) for \mathbb{I} between the ket and the bra in (12.25), and using $\int_0^\beta d\tau = \beta$ and $\int d\mathbf{x} = V$. This gives us an integral representation of the delta function,

$$\int_{0}^{\beta} d\tau \int d\mathbf{x} \exp\left\{-i(\omega_{n'} - \omega_{n})\tau + i(\mathbf{k'} - \mathbf{k}) \cdot \mathbf{x}\right\} = V\beta \ \delta(\mathbf{k} - \mathbf{k'})\delta_{nn'}.$$
 (12.26)

Similarly, we have the orthogonality relation

$$\langle \mathbf{x}, \tau | \mathbf{x}', \tau' \rangle = \delta(\mathbf{x} - \mathbf{x}')\delta(\tau - \tau').$$
(12.27)

Enforcing the consistency of inserting expression (12.23) in between the bra and the ket in (12.27), leads to the following integral for the delta function:

$$\frac{1}{V\beta} \sum_{\mathbf{k},n} \exp\left\{-i\omega_n(\tau - \tau') + i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')\right\} = \delta(\mathbf{x} - \mathbf{x}')\delta(\tau - \tau'). \quad (12.28)$$

Note the factor $1/(\beta V)$ in front of the summation. It is easy to check, by the way, that the definitions for the Fourier transform of the Grassmann variables in the previous paragraph are consistent with the definitions of the Fourier transforms given here. How do the fields transform under this? If we introduce $\Delta_{\mathbf{q},m} = \langle \mathbf{q}, m | \Delta \rangle$ and assume that $\Delta_{\mathbf{x},\tau} = \langle \mathbf{x}, \tau | \Delta \rangle$ then

$$\Delta_{\mathbf{x},\tau} = \sum_{\mathbf{q},m} \frac{e^{-i\varpi_m \tau + i\mathbf{q}\cdot\mathbf{x}}}{\sqrt{\beta V}} \,\Delta_{\mathbf{q},m} \tag{12.29}$$

$$\Leftrightarrow \Delta_{\mathbf{q},m} = \int_{0}^{\beta} d\tau \int d\mathbf{x} \; \frac{e^{i\boldsymbol{\varpi}_{m}\tau - i\mathbf{q}\cdot\mathbf{x}}}{\sqrt{\beta V}} \Delta_{\mathbf{x},\tau}.$$
 (12.30)

For the mind in need of consistency checks, note that substituting (12.29) in (12.30) gives back (12.28). And substituting (12.30) into (12.29) gives back (12.26). The same relations hold between $\psi_{\mathbf{x},\tau,\sigma}$ and $\psi_{\mathbf{k},n,\sigma}$ – we used those already in (12.16). We also introduce $\bar{\Delta}_{\mathbf{q},m} = \langle \Delta | \mathbf{q}, m \rangle$ and assume that $\bar{\Delta}_{\mathbf{x},\tau} = \langle \Delta | \mathbf{x}, \tau \rangle$, then we have

$$\bar{\Delta}_{\mathbf{x},\tau} = \sum_{\mathbf{q},m} \frac{e^{i\varpi_m \tau - i\mathbf{q}\cdot\mathbf{x}}}{\sqrt{\beta V}} \bar{\Delta}_{\mathbf{q},m}$$
(12.31)

$$\Leftrightarrow \bar{\Delta}_{\mathbf{q},m} = \int_{0}^{\beta} d\tau \int d\mathbf{x} \; \frac{e^{-i\varpi_{m}\tau + i\mathbf{q}\cdot\mathbf{x}}}{\sqrt{\beta V}} \bar{\Delta}_{\mathbf{x},\tau}.$$
 (12.32)

Also here we have the same relations linking $\bar{\psi}_{\mathbf{x},\tau,\sigma}$ and $\bar{\psi}_{\mathbf{k},n,\sigma}$, cf. expression (12.17). Note that here we have distributed the $\sqrt{\beta V}$ factors evenly over the Fourier and the inverse Fourier. As a result, we will have to tag a factor $\sqrt{\beta V}$ along later. If we keep the βV completely in the Fourier transform (12.32) or (12.30) then this does not appear.

Everything is now is set for the Fourier transformation of the partition function given in (12.20). The first term in the action of (12.20) is re-expressed with (12.31) and (12.29) as

$$\int_{0}^{\beta} d\tau \int d\mathbf{x} \ \bar{\Delta}_{\mathbf{x},\tau} \Delta_{\mathbf{x},\tau} = \int_{0}^{\beta} d\tau \int d\mathbf{x} \left(\sum_{\mathbf{q},m} \frac{e^{i\varpi_{m}\tau - i\mathbf{q}\cdot\mathbf{x}}}{\sqrt{\beta V}} \ \bar{\Delta}_{\mathbf{q},m} \right) \\
\times \left(\sum_{\mathbf{q}',m'} \frac{e^{-i\varpi_{m'}\tau + i\mathbf{q}'\cdot\mathbf{x}}}{\sqrt{\beta V}} \ \Delta_{\mathbf{q}',m'} \right) \\
= \sum_{\mathbf{q},m} \sum_{\mathbf{q}',m'} \left[\frac{1}{\beta V} \int_{0}^{\beta} d\tau \int d\mathbf{x} \ e^{i(\varpi_{m} - \varpi_{m'})\tau - i(\mathbf{q} - \mathbf{q}')\cdot\mathbf{x}} \right] \bar{\Delta}_{\mathbf{q},m} \Delta_{\mathbf{q}',m'} \\
= \sum_{\mathbf{q},m} \ \bar{\Delta}_{\mathbf{q},m} \Delta_{\mathbf{q},m}, \tag{12.33}$$

where we have used (12.26) in the last step. This is merely Parseval's rule.

Now we want to calculate the reciprocal space representation of the second part of the action in (12.20) given by

$$\int_{0}^{\beta} d\tau \int d\mathbf{x} \left[\bar{\eta}_{\mathbf{x},\tau} \cdot \left(-\mathbb{G}_{\mathbf{x},\tau}^{-1} \right) \cdot \eta_{\mathbf{x},\tau} \right] \\
= \int_{0}^{\beta} d\tau \int d\mathbf{x} \left(\bar{\psi}_{\mathbf{x},\tau,\uparrow} \left(\frac{\partial}{\partial \tau} - \nabla_{\mathbf{x}}^{2} - \mu_{\uparrow} \right) \psi_{\mathbf{x},\tau,\uparrow} + \psi_{\mathbf{x},\tau,\downarrow} \left(\frac{\partial}{\partial \tau} + \nabla_{\mathbf{x}}^{2} + \mu_{\downarrow} \right) \bar{\psi}_{\mathbf{x},\tau,\downarrow} \\
-\Delta_{\mathbf{x},\tau} \bar{\psi}_{\mathbf{x},\tau,\uparrow} \bar{\psi}_{\mathbf{x},\tau,\downarrow} - \bar{\Delta}_{\mathbf{x},\tau} \psi_{\mathbf{x},\tau,\downarrow} \psi_{\mathbf{x},\tau,\uparrow} \right).$$
(12.34)

Every term in (12.34) can be transformed to reciprocal space using the rules and conventions that we stated above. The first term in (12.34) becomes

$$\int_{0}^{\beta} d\tau \int d\mathbf{x} \ \bar{\psi}_{\mathbf{x},\tau,\uparrow} \left(\frac{\partial}{\partial \tau} - \nabla_{\mathbf{x}}^{2} - \mu_{\uparrow} \right) \psi_{\mathbf{x},\tau,\uparrow}
= \sum_{\mathbf{k},n} \sum_{\mathbf{k}',n'} \frac{1}{\beta V} \int_{0}^{\beta} d\tau \int d\mathbf{x} \ \left(e^{i\omega_{n}\tau - i\mathbf{k}.\mathbf{x}} \bar{\psi}_{\mathbf{k},n,\uparrow} \right)
\times \left(-i\omega_{n'} + (k')^{2} - \mu_{\uparrow} \right) \left(e^{-i\omega_{n'}\tau + i\mathbf{k}'.\mathbf{x}} \psi_{\mathbf{k}',n',\uparrow} \right)
= \sum_{\mathbf{k},n} \left(-i\omega_{n} + k^{2} - \mu_{\uparrow} \right) \bar{\psi}_{\mathbf{k},n,\uparrow} \psi_{\mathbf{k},n,\uparrow}.$$
(12.35)

The second term transforms completely analogously:

$$\int_{0}^{\beta} d\tau \int d\mathbf{x} \ \psi_{\mathbf{x},\tau,\downarrow} \left(\frac{\partial}{\partial \tau} + \nabla_{\mathbf{x}}^{2} + \mu_{\downarrow} \right) \bar{\psi}_{\mathbf{x},\tau,\downarrow}$$
$$= \sum_{\mathbf{k},n} \left(i\omega_{n} - k^{2} + \mu_{\downarrow} \right) \psi_{\mathbf{k},n,\downarrow} \bar{\psi}_{\mathbf{k},n,\downarrow}. \tag{12.36}$$

In the interaction terms, all three fields have to be transformed

$$-\int_{0}^{\beta} d\tau \int d\mathbf{x} \,\Delta_{\mathbf{x},\tau} \bar{\psi}_{\mathbf{x},\tau,\uparrow} \bar{\psi}_{\mathbf{x},\tau,\downarrow}$$

$$= -\frac{1}{\sqrt{\beta V}} \sum_{\mathbf{k},n} \sum_{\mathbf{k}',n'} \left[\frac{1}{\sqrt{\beta V}} \int_{0}^{\beta} d\tau \int d\mathbf{x} \left(e^{i(\omega_{n}+\omega_{n'})\tau - i\left(\mathbf{k}+\mathbf{k}'\right)\cdot\mathbf{x}} \Delta_{\mathbf{x},\tau} \right) \right] \bar{\psi}_{\mathbf{k},n,\uparrow} \bar{\psi}_{\mathbf{k}',n',\downarrow}$$

$$= -\frac{1}{\sqrt{\beta V}} \sum_{\mathbf{k},n} \sum_{\mathbf{k}',n'} \Delta_{\mathbf{k}+\mathbf{k}',n+n'} \bar{\psi}_{\mathbf{k},n,\uparrow} \bar{\psi}_{\mathbf{k}',n',\downarrow}, \qquad (12.37)$$

and analogously for the fourth term we arrive at

$$-\int_{0}^{\beta} d\tau \int d\mathbf{x} \ \bar{\Delta}_{\mathbf{x},\tau} \psi_{\mathbf{x},\tau,\downarrow} \psi_{\mathbf{x},\tau,\uparrow} = -\frac{1}{\sqrt{\beta V}} \sum_{\mathbf{k},n} \sum_{\mathbf{k}',n'} \ \bar{\Delta}_{\mathbf{k}+\mathbf{k}',n+n'} \ \psi_{\mathbf{k},n,\downarrow} \psi_{\mathbf{k}',n',\uparrow}.$$
(12.38)

In (12.37) and (12.38) we used (12.30) and (12.32) respectively, together with the fact that the sum of two fermionic Matsubara frequencies results in a bosonic Matsubara frequency. Putting all results together, the partition sum in reciprocal space equals

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}_{\mathbf{k},n,\sigma} \mathcal{D}\psi_{\mathbf{k},n,\sigma} \int \mathcal{D}\bar{\Delta}_{\mathbf{q},m} \mathcal{D}\Delta_{\mathbf{q},m} \exp\left(\sum_{\mathbf{q},m} \frac{\bar{\Delta}_{\mathbf{q},m} \Delta_{\mathbf{q},m}}{g} - \sum_{\mathbf{k}',n'} \sum_{\mathbf{k}'',n''} \bar{\eta}_{\mathbf{k}',n'} \langle \mathbf{k}',n'| - \mathbb{G}^{-1} |\mathbf{k}'',n'' \rangle \eta_{\mathbf{k}'',n''} \right),$$
(12.39)

where the reciprocal space representation of the inverse Green's function is given by:

$$\langle \mathbf{k}, n | - \mathbb{G}^{-1} | \mathbf{k}', n' \rangle = \langle \mathbf{k}, n | \mathbf{k}', n' \rangle \begin{pmatrix} -i\omega_n + k^2 - \mu_{\uparrow} & 0 \\ 0 & i\omega_n - k^2 + \mu_{\downarrow} \end{pmatrix}$$

$$+ \frac{1}{\sqrt{\beta V}} \begin{pmatrix} 0 & -\Delta_{\mathbf{k} + \mathbf{k}', n + n'} \\ -\bar{\Delta}_{\mathbf{k} + \mathbf{k}', n + n'} & 0 \end{pmatrix}.$$
(12.40)

where the following Nambu spinors were used

$$\eta_{\mathbf{k},n} = \begin{pmatrix} \psi_{\mathbf{k},n,\uparrow} \\ \bar{\psi}_{\mathbf{k},n,\downarrow} \end{pmatrix} \text{ en } \bar{\eta}_{\mathbf{k},n} = \begin{pmatrix} \bar{\psi}_{\mathbf{k},n,\uparrow} & \psi_{\mathbf{k},n,\downarrow} \end{pmatrix}.$$
(12.41)

Only the first part, the noninteracting part, is diagonal! The part related to the fermion pair field is not diagonal in reciprocal space, in the sense that components of the inverse Green's function with \mathbf{k}', n' different from \mathbf{k}, n are nonzero. Now we cannot use the result (12.12) since we have also have non-diagonal elements (i.e. between $\bar{\eta}_{\mathbf{k}',n'}$ and $\eta_{\mathbf{k}'',n''}$ with $\mathbf{k}'' \neq \mathbf{k}'$ and $n'' \neq n'$). In principle this is still a quadratic integral and we could do it, but it would involve taking a determinant (or logarithm) of $\langle \mathbf{k}', n' | - \mathbb{G}^{-1} | \mathbf{k}'', n'' \rangle$. This is a $\infty \times \infty$ matrix with 2×2 matrices as its elements. So let us postpone this horror, and see if we can get somewhere with approximations.

12.5 The Saddle Point Approximation

We have performed the Grassmann integrations, and even have obtained two equivalent expressions of the result, in position space and in reciprocal space. The result still contains a path integral over the bosonic pair fields $\bar{\Delta}_{\mathbf{q},m}, \Delta_{\mathbf{q},m}$, and this integral cannot be done analytically. Then why go through all the trouble of introducing these fields, and doing the fermionic integrals, if in the end we are left with another path integral that cannot be done exactly? The advantage of having rewritten the action into the form with the bosonic fields, is that we can use additional information about this bosonic pair field. Indeed, if we want to investigate the superfluid state, where the pairs are Bose condensed, we know that the field will be dominated by one contribution, that of the $\mathbf{q} = 0$ term. This is similar to the assumption of Bogoliubov in his famous treatment of the helium superfluid. In that case, Bogoliubov proposed to shift the bosonic operators over a $\mathbf{q} = 0$ contribution, so that the shifted operators could be seen as small fluctuations. This scheme is what we will apply now to treat the Bose fluid of pairs described by $\overline{\Delta}_{\mathbf{q},m}, \Delta_{\mathbf{q},m}$.

As mentioned, the simplest approximation is to assume all pairs are condensed in the $\mathbf{q} = 0$, m = 0 state and set for the two pair fields

$$\Delta_{\mathbf{q},m} = \sqrt{\beta V \delta(\mathbf{q})} \delta_{m,0} \times \Delta \tag{12.42}$$

$$\bar{\Delta}_{\mathbf{q},m} = \sqrt{\beta V \delta(\mathbf{q})} \delta_{m,0} \times \Delta^*. \tag{12.43}$$

We introduce the factor $\sqrt{\beta V}$ for the ease of calculation and to give Δ units of energy. By applying the saddle point (12.42) and (12.43) the partition function becomes

$$\begin{aligned} \mathcal{Z}_{sp} &= \int \mathcal{D}\bar{\psi}_{\mathbf{k},n,\sigma} \mathcal{D}\psi_{\mathbf{k},n,\sigma} \exp\left(\frac{\beta V}{g} \left|\Delta\right|^2 - \sum_{\mathbf{k},n} \left(-i\omega_n + k^2 - \mu_{\uparrow}\right) \bar{\psi}_{\mathbf{k},n,\uparrow} \psi_{\mathbf{k},n,\uparrow} \right. \\ &\left. - \sum_{\mathbf{k},n} \left(-i\omega_n - k^2 + \mu_{\downarrow}\right) \psi_{\mathbf{k},-n,\downarrow} \bar{\psi}_{\mathbf{k},-n,\downarrow} \right. \\ &\left. + \sum_{\mathbf{k},n} \left(\Delta \bar{\psi}_{\mathbf{k},n,\uparrow} \bar{\psi}_{-\mathbf{k},-n,\downarrow} + \Delta^* \psi_{-\mathbf{k},-n,\downarrow} \psi_{\mathbf{k},n,\uparrow}\right)\right). \end{aligned}$$
(12.44)

We explicitly write out the action without Nambu spinors here to make an important and subtle point, which otherwise is quickly overlooked. The alert reader will have noticed that we have re-indexed the indices in the spin-down two-particle term. This re-indexation is necessary in order to write the action in Nambu spinor notation. Here the following Nambu spinors will be used

$$\eta_{\mathbf{k},n} = \begin{pmatrix} \psi_{\mathbf{k},n,\uparrow} \\ \bar{\psi}_{-\mathbf{k},-n,\downarrow} \end{pmatrix} \text{ en } \bar{\eta}_{\mathbf{k},n} = \begin{pmatrix} \bar{\psi}_{\mathbf{k},n,\uparrow} & \psi_{-\mathbf{k},-n,\downarrow} \end{pmatrix}.$$
(12.45)

This then leads to the inverse Green's function in the saddle-point approximation

$$\langle \mathbf{k}', n' | - \mathbb{G}_{sp}^{-1} | \mathbf{k}, n \rangle = \langle \mathbf{k}, n | \mathbf{k}', n' \rangle \begin{pmatrix} -i\omega_n + k^2 - \mu_{\uparrow} & -\Delta \\ -\Delta^* & -i\omega_n - k^2 + \mu_{\downarrow} \end{pmatrix}$$
$$= \langle \mathbf{k}, n | \mathbf{k}', n' \rangle \quad \left(-\mathbb{G}_{sp}^{-1} \right)'_{\mathbf{k}, n}.$$
(12.46)

Our choice has made the inverse Green's function diagonal, since none of the terms $\Delta_{\mathbf{k}'+\mathbf{k},n'+n}$ with $\mathbf{k}'+\mathbf{k}\neq\mathbf{0}$ or $n'+n\neq0$ survive due to the delta functions in (12.42), and similarly for $\overline{\Delta}$. Note the sign change of the term $i\omega_n$ in the lower right part of (12.46) which arises because of a re-indexation of

In the saddle-point approximation to the partition sum we no longer have to perform the integrations over the bosonic degrees (it is this integration which was approximated):

$$\mathcal{Z}_{sp} = \int \mathcal{D}\bar{\psi}_{\mathbf{k},n,\sigma} \mathcal{D}\psi_{\mathbf{k},n,\sigma} \exp\left\{\frac{\beta V}{g} \left|\Delta\right|^2 - \sum_{\mathbf{k},n} \bar{\eta}_{\mathbf{k},n} \cdot \left(-\mathbb{G}_{sp}^{-1}\right) \cdot \eta_{\mathbf{k},n}\right\}.$$
 (12.47)

We can now perform the Grassmann integration:

$$\int \mathcal{D}\bar{\psi}_{\mathbf{k},n,\sigma} \mathcal{D}\psi_{\mathbf{k},n,\sigma} \exp\left\{-\sum_{\mathbf{k},n} \bar{\eta}_{\mathbf{k},n} \cdot \left(-\mathbb{G}_{sp}^{-1}\right)_{\mathbf{k},n} \cdot \eta_{\mathbf{k},n}\right\}$$
$$= \exp\left\{\sum_{\mathbf{k},n} \ln\left[-\det_{\sigma}\left(-\mathbb{G}_{sp}^{-1}\right)_{\mathbf{k},n}\right]\right\}.$$
(12.48)

12.5. THE SADDLE POINT APPROXIMATION

This spinor-determinant is given by

$$-\det_{\sigma} \left(-\mathbb{G}_{sp}^{-1}\right)_{\mathbf{k},n} = -\det \left(\begin{array}{cc} -i\omega_n + k^2 - \mu_{\uparrow} & -\Delta \\ -\Delta^* & -i\omega_n - k^2 + \mu_{\downarrow} \end{array}\right)$$
$$= -\left(-i\omega_n + k^2 - \mu_{\uparrow}\right) \left(-i\omega_n - k^2 + \mu_{\downarrow}\right) + |\Delta|^2 \,. \quad (12.49)$$

Introducing

$$\mu = (\mu_{\uparrow} + \mu_{\downarrow})/2, \qquad (12.50)$$

$$\zeta = (\mu_{\uparrow} - \mu_{\downarrow})/2, \tag{12.51}$$

$$E_{\mathbf{k}} = \sqrt{\left(k^2 - \mu\right)^2 + \left|\Delta\right|^2},$$
 (12.52)

we can rewrite this as

$$-\det_{\sigma} \left(-\mathbb{G}_{sp}^{-1} \right)_{\mathbf{k},n} = \left(i\omega_n + \zeta - E_{\mathbf{k}} \right) \left(-i\omega_n - \zeta - E_{\mathbf{k}} \right).$$
(12.53)

This can easily be checked by substituting and seeing that both expressions are indeed equal (and equal to $\omega_n^2 + (k^2 - \mu)^2 + |\Delta|^2 - \zeta^2 - 2i\omega_n\zeta$). So, the saddle-point partition sum becomes

$$\mathcal{Z}_{sp} = \exp\left\{\frac{\beta V}{g} \left|\Delta\right|^2 + \sum_{\mathbf{k},n} \ln\left[\left(i\omega_n + \zeta - E_{\mathbf{k}}\right)\left(-i\omega_n - \zeta - E_{\mathbf{k}}\right)\right]\right\}.$$
 (12.54)

The partition function is also linked to the thermodynamic potential through the well-known formula

$$\mathcal{Z}_{sp} = e^{-\beta F_{sp}(T, V, \mu_{\uparrow}, \mu_{\downarrow})}.$$
(12.55)

Note that this is the free energy as a function of the chemical potentials. It is related to the usual free energy through

$$F(T, V, \mu_{\uparrow}, \mu_{\downarrow}) = F(T, V, N_{\uparrow}, N_{\downarrow}) - \mu_{\uparrow} N_{\uparrow} - \mu_{\downarrow} N_{\downarrow}$$
(12.56)

with
$$\begin{cases} N_{\uparrow} = -\frac{\partial F(T, V, \mu_{\uparrow}, \mu_{\downarrow})}{\partial \mu_{\uparrow}} \Big|_{T, V, \mu_{\downarrow}} \\ N_{\downarrow} = -\frac{\partial F(T, V, \mu_{\uparrow}, \mu_{\downarrow})}{\partial \mu_{\downarrow}} \Big|_{T, V, \mu_{\uparrow}} \end{cases}$$
(12.57)

or, in μ and ζ :

$$F(T, V, \mu, \zeta) = F(T, V, N, \delta N) - \mu N - \zeta \delta N, \qquad (12.58)$$

where $N = N_{\uparrow} + N_{\downarrow}$ and $\delta N = N_{\uparrow} - N_{\downarrow}$. *F* is commonly referred to as the "thermodynamic potential". In following notations, we use $\Omega(T, V, \mu, \zeta) = F(T, V, \mu, \zeta)/V$ for the thermodynamic potential *per unit volume*,

$$\Omega(T, V, \mu, \zeta) = \frac{1}{V} F(T, V, N, \delta N) - \mu n - \zeta \delta n,$$

where n = N/V and $\delta n = \delta N/V$ are the total density and the density difference

$$n = -\left. \frac{\partial \Omega(T, V, \mu, \zeta)}{\partial \mu} \right|_{T, V, \zeta}$$
(12.59)

$$\delta n = - \left. \frac{\partial \Omega(T, V, \mu, \zeta)}{\partial \zeta} \right|_{T, V, \mu}.$$
(12.60)

We give these expressions explicitly here to avoid the subtle difficulties related to identifying the dependent variables. For the saddle-point action we get:

$$\mathcal{Z}_{sp} = e^{-\beta V \Omega_{sp}(T,\mu,\zeta)}.$$
(12.61)

We dropped the explicit dependence on V because it also drops from the expression for Ω_{sp} . From (12.54) we get the saddle-point thermodynamic potential per unit volume

$$\Omega_{sp}(T,\mu,\zeta) = -\frac{1}{g} |\Delta|^2 - \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{\beta} \sum_{n} \ln\left[\left(i\omega_n + \zeta - E_{\mathbf{k}}\right)\left(-i\omega_n - \zeta - E_{\mathbf{k}}\right)\right].$$
(12.62)

Note that since the density of **k**-states in reciprocal space is $V/(2\pi)^3$ we can replace

$$\frac{1}{V}\sum_{\mathbf{k}} \to \int \frac{d^3\mathbf{k}}{(2\pi)^3}.$$
(12.63)

We do not have to take the Matsubara sums now. For example we might want to take derivatives first.

In the sum over Matsubara frequencies we sum up terms with all $n \in \mathbb{Z}$. We can re-order the terms in this sum. In particular, we can set n' = -1 - n and sum over all n'. For this substitution $i\omega_{n'} = i\omega_{-n-1} = -i\omega_n$. This means that in a general Matsubara summation

$$\frac{1}{\beta}\sum_{n=-\infty}^{\infty}f(i\omega_n) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty}f(-i\omega_n)$$
(12.64)

must hold. With this we can transform the argument of the logarithm into $(-i\omega_n - \zeta - E_k)(i\omega_n + \zeta - E_k)$. Introducing

$$i\nu_n = i\omega_n + \zeta \tag{12.65}$$

as shifted Matsubara frequencies, and $\xi_{\mathbf{k}} = k^2 - \mu$, we get

$$\Omega_{sp}(T,\mu,\zeta;\Delta) = -\frac{1}{g} |\Delta|^2 - \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \left\{ \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \ln\left[-\left(i\nu_n + E_{\mathbf{k}}\right)\left(i\nu_n - E_{\mathbf{k}}\right)\right] - \xi_{\mathbf{k}} \right\}$$
(12.66)

We use this notation to make an important point. The thermodynamic potential per unit volume Ω_{sp} will depend on our choice of saddle-point value, but this

is not one of the thermodynamic variables like T, μ and ζ . If we want to treat Δ as a separate input for Ω_{sp} , we will write this as $\Omega_{sp}(T, \mu, \zeta; \Delta)$ to emphasize the distinction between Δ and the true thermodynamic variables. We extract the dependence of Δ on the thermodynamic variables from the gap equation

$$\frac{\partial\Omega_{sp}(T,\mu,\zeta;\Delta)}{\partial\Delta}\bigg|_{T,\mu,\zeta} = 0 \quad \longrightarrow \quad \Delta(T,\mu,\zeta)$$

and we have to insert this result back into $\Omega_{sp}(T,\mu,\zeta;\Delta(T,\mu,\zeta)) = \Omega_{sp}(T,\mu,\zeta)$ when applying thermodynamic relations. For example, the number equations are given by the thermodynamic relations

$$n_{sp} = -\left. \frac{\partial \Omega_{sp}(T,\mu,\zeta)}{\partial \mu} \right|_{T,\zeta}$$
(12.67)

$$\delta n_{sp} = -\left. \frac{\partial \Omega_{sp}(T,\mu,\zeta)}{\partial \zeta} \right|_{T,\mu}.$$
(12.68)

If we want to treat Δ as a separate variable then we need to use the chain rule

$$n_{sp} = -\left. \frac{\partial \Omega_{sp} \left[T, \mu, \zeta; \Delta \right]}{\partial \mu} \right|_{T,\zeta,\Delta} - \left. \frac{\partial \Omega_{sp} \left[T, \mu, \zeta; \Delta \right]}{\partial \Delta} \right|_{T,\zeta,\mu} \times \left. \frac{\partial \Delta(T, \mu, \zeta)}{\partial \mu} \right|_{T,\zeta}.$$
(12.69)

Now you might wonder what all the fuss is about, since we just imposed

$$\frac{\partial\Omega_{sp}\left[T,\mu,\zeta;\Delta\right]}{\partial\Delta}\bigg|_{T,\zeta,\mu} = 0, \qquad (12.70)$$

so that here

$$n_{sp} = -\left. \frac{\partial \Omega_{sp} \left[T, \mu, \zeta; \Delta \right]}{\partial \mu} \right|_{T,\zeta,\Delta}.$$
(12.71)

We have been cautious with the partial derivatives and thermodynamic relations, and this might seem superfluous for the saddle-point approximation, but it will become very important when we are adding fluctuation corrections to the thermodynamic potential.

12.6 Thermodynamic grand potential

To obtain the results at the saddle-point level, we need to perform the Matsubara summations in the thermodynamic potential:

$$\frac{1}{\beta}\sum_{n=-\infty}^{\infty}\ln\left[-(i\nu_n-E)(i\nu_n+E)\right] = \frac{1}{\beta}\ln\left[2\cosh(\beta E_{\mathbf{k}}) + 2\cosh(\beta\zeta)\right] + \sum_{\substack{n=-\infty\\(12.72)}}^{\infty}\ln\left(\nu_n^2\right)$$

Due to the presence of the logarithm this Matsubara sum is divergent. Luckily however, the divergent part, which does not depend on the system parameters, can be neatly isolated, as shown in (12.72). This means that the free energy can be regularized by subtracting this unphysical term. This then results in:

$$\Omega_{sp}(T,\mu,\zeta;\Delta) = -\frac{1}{g} |\Delta|^2 - \frac{1}{V} \sum_{\mathbf{k}} \left\{ \frac{1}{\beta} \ln\left[2\cosh(\beta E_{\mathbf{k}}) + 2\cosh(\beta\zeta)\right] - \xi_{\mathbf{k}} \right\}.$$
(12.73)

Using the renormalized contact potential strength, this becomes

$$\Omega_{sp}(T,\mu,\zeta;\Delta) = -\frac{1}{8\pi k_F a_s} |\Delta|^2 \qquad (12.74)$$
$$-\frac{1}{V} \sum_{\mathbf{k}} \left\{ \frac{1}{\beta} \ln\left[2\cosh(\beta E_{\mathbf{k}}) + 2\cosh(\beta \zeta)\right] - \xi_{\mathbf{k}} - \frac{|\Delta|^2}{2k^2} \right\}.$$

We kept $(k_F a_s)$ as the measure of interaction strength, explicitly writing k_F although we have used it as a length unit, as if $(k_F a_s)$ were a single symbol for the interaction strength. In three dimensions, this is reduced to

$$\Omega_{sp}(T,\mu,\zeta;\Delta) = -\frac{1}{8\pi k_F a_s} |\Delta|^2$$

$$-\int \frac{d\mathbf{k}}{(2\pi)^3} \left\{ \frac{1}{\beta} \ln\left[2\cosh(\beta E_{\mathbf{k}}) + 2\cosh(\beta\zeta)\right] - \xi_{\mathbf{k}} - \frac{|\Delta|^2}{2k^2} \right\}.$$
(12.75)

Since we have isotropy, this is

$$\Omega_{sp}(T,\mu,\zeta;\Delta) = -\frac{1}{8\pi k_F a_s} |\Delta|^2$$

$$-\frac{1}{2\pi^2} \int_0^\infty dk \ k^2 \left\{ \frac{1}{\beta} \ln\left[2\cosh(\beta E_{\mathbf{k}}) + 2\cosh(\beta\zeta)\right] - \xi_{\mathbf{k}} - \frac{|\Delta|^2}{2k^2} \right\}.$$
(12.76)

This result is shown in figure 12.2.

In the limit of low temperature we have a simplification:

$$\lim_{\beta \to \infty} \frac{1}{\beta} \ln \left[2 \cosh(\beta E_{\mathbf{k}}) + 2 \cosh(\beta \zeta) \right] = \max \left(E_k, |\zeta| \right).$$
(12.77)

Also note that in the limit of large k, the logarithm behaves as

$$\lim_{k \to \infty} \ln \left[2 \cosh(\beta E_{\mathbf{k}}) + 2 \cosh(\beta \zeta) \right] = \xi_{\mathbf{k}} + \frac{|\Delta|^2}{2k^2} + \mathcal{O}(k^{-4}), \quad (12.78)$$

so that it is precisely the extra terms $\xi_{\mathbf{k}} + |\Delta|^2 / (2k^2)$ that keep the integrand from diverging and keep the saddle-point free energy that we calculate here finite. Remember that $\xi_{\mathbf{k}} = (k^2 - \mu)$ and $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$.

From this result, and from

$$\frac{\partial E_k}{\partial \Delta} = \frac{\Delta}{E_k}$$



Figure 12.2: The saddle-point free energy per unit volume is shown as a function of the gap parameter Δ , for different values of the imbalance chemical potential ζ , at temperature $T/T_F = 0.01$ and average chemical potential $\mu = 1.3$. As the imbalance chemical potential ζ is increased, the normal state minimum at $\Delta = 0$ develops and becomes the global minimum above a critical imbalance level. The superfluid state minimum at $\Delta \neq 0$ is not influenced by ζ , indicating that the superfluid state is balanced, i.e. has an equal amount of spin-up and spin-down components. The excess component in this state must be expelled, leading to phase separation.

we can obtain the gap equation:

$$\frac{\partial\Omega_{sp}}{\partial\Delta} = 0$$

$$\iff -\frac{1}{k_F a_s} = \frac{2}{\pi} \int_0^\infty dk \left[\frac{\sinh(\beta E_k)}{\cosh(\beta E_k) + \cosh(\beta \zeta)} \frac{k^2}{E_k} - 1 \right]. \quad (12.79)$$

For every temperature and every μ, ζ , this equation can be solved to obtain $\Delta_{sp}(T, \mu, \zeta)$, the value of Δ that indeed minimizes Ω_{sp} (as can be checked from the sign of the second derivative, or by visual inspection of the plot of Ω_{sp} as a function of Δ at fixed T, μ, ζ). The resulting saddle point gap is illustrated in figure 12.3.

The presence of imbalance $(\zeta \neq 0)$ only affects the energies $E_{\mathbf{k}} < \zeta$ in the temperature zero limit, since in that limit

$$\lim_{\beta \to \infty} \frac{\sinh\left(\beta E_{\mathbf{k}}\right)}{\cosh\left(\beta \zeta\right) + \cosh\left(\beta E_{\mathbf{k}}\right)} \to \begin{cases} 1 \text{ for } |\zeta| < E_{\mathbf{k}} \\ 0 \text{ for } |\zeta| > E_{\mathbf{k}} \end{cases}$$
(12.80)

The presence of a gap results in $E_{\mathbf{k}} > \Delta$. Thus, as long as $\zeta < \Delta$, the imbalance (at T=0) will not affect the gap equation, and we retrieve the Clogston limit for superconductivity. This argument is only valid in the BCS limit, because



Figure 12.3: The value of the gap parameter that minimizes the saddle-point free energy is shown as a function of the interaction strength $1/(k_F a_s)$. In the limit of $(k_F a_s)^{-1} \rightarrow -\infty$, the Bardeen-Cooper-Schrieffer (BCS) result is retrieved, whereas in the limit of $(k_F a_s)^{-1} \rightarrow +\infty$, a Bose-Einstein condensate (BEC) of tightly bound Cooper pairs is formed. The different curves show the effect of increasing the temperature: the BCS state is more strongly affected than the BEC state. However, in the BEC state, phase fluctuations (discussed in the next sections) will become the dominant mechanism to destroy superfluidity, rather than the breakup of the Cooper pairs as in BCS.



Figure 12.4: The value of the gap parameter that minimizes the saddle-point free energy is shown as a function of the interaction strength $1/(k_Fa_s)$, as in figure 12.3. In the current figure, the different curves correspond to different values of the imbalance chemical potential ζ . At the saddle-point level, it becomes clear that introducing imbalance between 'spin-up' and 'spin-down' components leads to the appearance of a critical interaction parameter below which pairing is suppressed.

for the BEC/BCS crossover we still need to solve (independently) the number equation that is coupled to the gap equation. Results for this are illustrated in figure 12.4. Only in the BCS limit we can set $\mu = E_F$ and not worry about the overall chemical potential further.

When working with a fixed number of particles, the chemical potentials need to be related to these numbers of particles through the number equations. These are again found from the thermodynamic potential, and from

$$-\frac{\partial E_k}{\partial \mu} = \frac{\xi_k}{E_k} \tag{12.81}$$

we get

$$n_{sp} = -\frac{\partial\Omega_{sp}\left[T,\mu,\zeta;\Delta\right]}{\partial\mu}\bigg|_{T,\zeta,\Delta}$$
$$= \frac{1}{2\pi^2} \int_{0}^{\infty} dk \ k^2 \left\{ 1 - \frac{\sinh(\beta E_k)}{\cosh(\beta E_k) + \cosh(\beta \zeta)} \frac{\xi_k}{E_k} \right\}$$
(12.82)

and

$$\delta n_{sp} = - \left. \frac{\partial \Omega_{sp} \left[T, \mu, \zeta; \Delta \right]}{\partial \zeta} \right|_{T,\mu,\Delta} = \frac{1}{2\pi^2} \int_0^\infty dk \ k^2 \frac{\sinh(\beta\zeta)}{\cosh(\beta E_k) + \cosh(\beta\zeta)}.$$
(12.83)

Now note that we did indeed work at a fixed number of particles from the start, in introducing our units $k_F = (3\pi^2 n)^{1/3}$. Hence, these two number equations become

$$\frac{1}{3\pi^2} = \frac{1}{2\pi^2} \int_0^\infty dk \ k^2 \left\{ 1 - \frac{\sinh(\beta E_k)}{\cosh(\beta E_k) + \cosh(\beta \zeta)} \frac{\xi_k}{E_k} \right\}$$
(12.84)

$$\frac{1}{3\pi^2} \frac{\delta n_{sp}}{n_{sp}} = \frac{1}{2\pi^2} \int_0^\infty dk \ k^2 \frac{\sinh(\beta\zeta)}{\cosh(\beta E_k) + \cosh(\beta\zeta)}$$
(12.85)

and we have to solve the gap equation in conjunction with these two number equations: all three have to be satisfied. The third one can be solved and merely fixes ζ as a function of δn_{sp} , but the first number equation together with the gap equation are coupled in the two remaining unknowns μ , Δ . Solutions for Δ are shown in figures 12.3 and 12.4. Figure 12.5 shows results for the chemical potential.

12.7 Partition sum phase factor

Before we look at fluctuations beyond mean field, there is an important remark to be made: we can no longer delay looking at non-diagonal Gaussian integrations. Remember, when we do not restrict ourselves to the saddle-point value, we need to evaluate (see Eq. (12.39))

$$\int \mathcal{D}\bar{\psi}_{\mathbf{k},n,\sigma} \mathcal{D}\psi_{\mathbf{k},n,\sigma} \exp\left\{-\sum_{\mathbf{k},n} \sum_{\mathbf{k}',n'} \bar{\eta}_{\mathbf{k}',n'} \cdot \langle \mathbf{k}',n' | -\mathbb{G}^{-1} | \mathbf{k},n \rangle \cdot \eta_{\mathbf{k},n}\right\} \\
= \left[\prod_{\mathbf{k},n} (-1)\right] \int \mathcal{D}\bar{\eta}_{\mathbf{k},n} \mathcal{D}\eta_{\mathbf{k},n} \exp\left\{-\sum_{\mathbf{k},n} \sum_{\mathbf{k}',n'} \bar{\eta}_{\mathbf{k}',n'} \cdot \langle \mathbf{k}',n' | -\mathbb{G}^{-1} | \mathbf{k},n \rangle \cdot \eta_{\mathbf{k},n}\right\} \tag{12.86}$$

Remember that the factors (-1) are coming from the change in integration measure. To keep track of it, we will give it its own symbol

$$\mathcal{X} = \prod_{\mathbf{k},n} \left(-1 \right).$$



Figure 12.5: The chemical potential μ is shown as a function of the interaction parameter $1/(k_F a_s)$, for a low temperature and a balanced gas ($\zeta = 0$). In the regime of negative a_s the chemical potential tends to the Fermi energy, as in the BCS theory. For positive a_s , the chemical potential tends to the binding energy of the strongly bound 'Cooper molecules' that Bose-Einstein condense to form a superfluid.

The matrix $\langle \mathbf{k}', n' | - \mathbb{G}^{-1} | \mathbf{k}, n \rangle$ has rows and columns indexed by \mathbf{k}, n and \mathbf{k}', n' . Each element in the matrix is itself a 2 × 2 matrix, and we could think of $\langle \mathbf{k}', n' | - \mathbb{G}^{-1} | \mathbf{k}, n \rangle = \mathbb{A}_{\mathbf{k}', n'; \mathbf{k}, n}$ as an $N \times N$ 'metamatrix' of matrices.

On the other hand, we could consider $-\mathbb{G}^{-1}$ as a $2N \times 2N$ matrix of scalars, indexed by \mathbf{k}, n, j where j = 1, 2 index the spinor components. That way we the Nambu integral is just a standard gaussian Grassmann integration. We could solve it by diagonalizing the $2N \times 2N$ matrix $-\mathbb{G}^{-1}$ with some $2N \times 2N$ unitary transformation matrix to prove

$$\int \mathcal{D}\bar{\eta}_{\mathbf{k},n} \mathcal{D}\eta_{\mathbf{k},n} \exp\left\{-\sum_{\mathbf{k},n,j} \sum_{\mathbf{k}',n',j'} \bar{\eta}_{\mathbf{k}',n',j'} \left(-\mathbb{G}^{-1}\right)_{\mathbf{k}',n',j';\mathbf{k},n,j} \eta_{\mathbf{k},n,j}\right\}$$
$$= \det\left(-\mathbb{G}^{-1}\right), \qquad (12.87)$$

where the determinant is now of the $2N \times 2N$ matrix. More matrix trickery is coming. We start innocently, by claiming

$$\det\left(-\mathbb{G}^{-1}\right) = \exp\left\{\ln\left[\det\left(-\mathbb{G}^{-1}\right)\right]\right\}$$
(12.88)

Now, remember that

- The determinant of any matrix is equal to the product of its eigenvalues.
- The logarithm of an $2N \times 2N$ matrix \mathbb{B} is another $2N \times 2N$ matrix \mathbb{C} such that $\mathbb{B} = \exp(\mathbb{C}) = \mathbb{I} + \sum_{n=1}^{\infty} (\mathbb{C})^n / n!$.
- The logarithm of a diagonal matrix is a diagonal matrix with the logarithm of the diagonal elements.

From these statements it can be shown that the logarithm of the determinant of a matrix equals the trace of the logarithm of the matrix. In other words

$$\ln\left[\det\left(-\mathbb{G}^{-1}\right)\right] = \operatorname{Tr}\left[\ln\left(-\mathbb{G}^{-1}\right)\right], \qquad (12.89)$$

where the trace is taken over all \mathbf{k}, n, j values. Combining (12.87) with (12.88) and (12.89), we get

$$\int \mathcal{D}\bar{\psi}_{\mathbf{k},n,\sigma} \mathcal{D}\psi_{\mathbf{k},n,\sigma} \exp\left\{-\sum_{\mathbf{k},n}\sum_{\mathbf{k}',n'} \bar{\eta}_{\mathbf{k}',n'} \cdot \langle \mathbf{k}',n' | -\mathbb{G}^{-1} | \mathbf{k},n \rangle \cdot \eta_{\mathbf{k},n}\right\}$$
$$= \mathcal{X} \exp\left\{\operatorname{Tr}\left[\ln\left(-\mathbb{G}^{-1}\right)\right]\right\}.$$
(12.90)

Expression (12.90) allows to write compactly the result of doing the Grassmann integrations in (12.39) and obtain the following exact result

$$\mathcal{Z} = \mathcal{X} \int \mathcal{D}\bar{\Delta}_{\mathbf{q},m} \mathcal{D}\Delta_{\mathbf{q},m} \exp\left\{\sum_{\mathbf{q},m} \frac{\bar{\Delta}_{\mathbf{q},m} \Delta_{\mathbf{q},m}}{g} + \operatorname{Tr}\left[\ln\left(-\mathbb{G}^{-1}\right)\right]\right\}.$$
 (12.91)
Replacing $-\mathbb{G}^{-1}$ by $-\mathbb{G}_{sp}^{-1}$ gives back the saddle-point result,

$$\mathcal{Z}_{sp} = \mathcal{X} \exp\left\{\frac{\beta V \left|\Delta\right|^2}{g} + \operatorname{Tr}\left[\ln\left(-\mathbb{G}_{sp}^{-1}\right)\right]\right\}.$$
 (12.92)

12.8 Fluctuations beyond mean field

12.8.1 Fluctuation expansion

If we want to improve on the saddle-point solution, we set

$$\Delta_{\mathbf{q},m} = \sqrt{\beta V} \delta(\mathbf{q}) \delta_{m,0} \Delta + \phi_{\mathbf{q},\mathbf{m}}$$
(12.93)

$$\bar{\Delta}_{\mathbf{q},m} = \sqrt{\beta V \delta(\mathbf{q})} \delta_{m,0} \Delta^* + \bar{\phi}_{\mathbf{q},\mathbf{m}}.$$
(12.94)

This is like the Bogoliubov shift in the second quantized theory of helium or Bose gases. We have a condensate contribution $\propto \Delta$ and add to it small fluctuations $\phi_{\mathbf{q},\mathbf{m}}$. Then we will expand up to second order in the fluctuations $\phi_{\mathbf{q},\mathbf{m}}, \overline{\phi}_{\mathbf{q},\mathbf{m}}$ and get a quadratic (bosonic) path integral that we can perform exactly. This line summarized the long tough program ahead in a single sentence.

We can choose our fluctuations around the saddle point differently. Rather than using two conjugate fields, we can choose to vary amplitude and phase, and employ fields $|\phi|_{\mathbf{q},m} e^{i\theta_{\mathbf{q},m}}$ so that

$$\Delta_{\mathbf{q},m} = \sqrt{\beta V} \delta(\mathbf{q}) \delta_{m,0} \Delta + |\phi|_{\mathbf{q},m} e^{i\theta_{\mathbf{q},m}}$$
$$\bar{\Delta}_{\mathbf{q},m} = \sqrt{\beta V} \delta(\mathbf{q}) \delta_{m,0} \Delta^* + |\phi|_{\mathbf{q},m} e^{-i\theta_{\mathbf{q},m}}.$$

This leads to a hydrodynamic description as a function of the density of fluctuations and the phase field. Basically this is a change in the integration variables representing the Gaussian fluctuation contribution to the free energy, and we expect the same results. We will work here with (12.93) and (12.94). Plugging this into the expression (12.40) for the inverse Green's function we can write

$$-\mathbb{G}^{-1} = -\mathbb{G}_{sp}^{-1} + \mathbb{F},\tag{12.95}$$

with like before, a diagonal piece for the saddle-point contribution,

$$\left\langle \mathbf{k}', n' \left| -\mathbb{G}_{sp}^{-1} \right| \mathbf{k}, n \right\rangle = \left\langle \mathbf{k}, n \right| \mathbf{k}', n' \right\rangle \begin{pmatrix} -i\omega_n + k^2 - \mu_{\uparrow} & -\Delta \\ -\Delta^* & -i\omega_n - k^2 + \mu_{\downarrow} \end{pmatrix}$$
(12.96)

and now the additional piece

$$\langle \mathbf{k}', n' | \mathbb{F} | \mathbf{k}, n \rangle = \frac{1}{\sqrt{\beta V}} \begin{pmatrix} 0 & -\phi_{\mathbf{k}'-\mathbf{k},n'-n} \\ -\bar{\phi}_{\mathbf{k}-\mathbf{k}',n-n'} & 0 \end{pmatrix}.$$
 (12.97)

Here again the change in sign in the index of the ϕ terms $\bar{\phi}_{\mathbf{k}-\mathbf{k}',n-n'} \rightarrow \bar{\phi}_{\mathbf{k}+\mathbf{k}',n+n'}$ is due to a re-indexation of the **k** and *n* indices, similar to expression (12.44). Now we are ready to expand $\ln(-\mathbb{G}^{-1})$ in the exact expression (12.91) for the partition function, using matrix algebra

$$\ln \left(-\mathbb{G}^{-1}\right) = \ln \left(-\mathbb{G}_{sp}^{-1} + \mathbb{F}\right)$$
$$= \ln \left[-\mathbb{G}_{sp}^{-1} + \mathbb{G}_{sp}^{-1}\mathbb{G}_{sp}\mathbb{F}\right]$$
$$= \ln \left[-\mathbb{G}_{sp}^{-1} \left(\mathbb{I} - \mathbb{G}_{sp}\mathbb{F}\right)\right]$$
$$= \ln \left(-\mathbb{G}_{sp}^{-1}\right) + \ln \left(\mathbb{I} - \mathbb{G}_{sp}\mathbb{F}\right).$$
(12.98)

So, the result for the (quadratic approximation to the) partition sum using the "Bogoliubov shifted fields" becomes

$$\begin{aligned} \mathcal{Z}_{q} &= \mathcal{X} \int \mathcal{D}\bar{\phi}_{\mathbf{q},m} \mathcal{D}\phi_{\mathbf{q},m} \exp\left\{\sum_{\mathbf{q},m} \frac{1}{g} \left(\sqrt{\beta V} \Delta^{*} \delta(\mathbf{q}) \delta_{m,0} + \bar{\phi}_{\mathbf{q},m}\right) \right. \\ & \left. \times \left(\sqrt{\beta V} \Delta \delta(\mathbf{q}) \delta_{m,0} + \phi_{\mathbf{q},m}\right) \right. \\ & \left. + \operatorname{Tr}\left[\ln\left(-\mathbb{G}_{sp}^{-1}\right)\right] + \operatorname{Tr}\left[\ln\left(\mathbb{I} - \mathbb{G}_{sp}\mathbb{F}\right)\right] \right\}. \end{aligned}$$
(12.99)

We can bring all the stuff that does not depend on the fluctuations in front of the integrals

$$\mathcal{Z}_{q} = \mathcal{X} \exp\left\{\frac{\beta V \left|\Delta\right|^{2}}{g} + \operatorname{Tr}\left[\ln\left(-\mathbb{G}_{sp}^{-1}\right)\right]\right\}$$
$$\times \int \mathcal{D}\bar{\phi}_{\mathbf{q},m} \mathcal{D}\phi_{\mathbf{q},m} \exp\left\{\frac{\sqrt{\beta V}}{g}\left(\Delta^{*}\phi_{\mathbf{0},0} + \Delta\bar{\phi}_{\mathbf{0},0}\right) + \sum_{\mathbf{q},m}\frac{\bar{\phi}_{\mathbf{q},m}\phi_{\mathbf{q},m}}{g} + \operatorname{Tr}\left[\ln\left(\mathbb{I} - \mathbb{G}_{sp}\mathbb{F}\right)\right]\right\}.$$
(12.100)

The factor on the first line is nothing else but \mathcal{Z}_{sp} , expression (12.92). This absorbs the nasty factor \mathcal{X} and results in $\exp\{-\beta V \Omega_{sp}\}$.

Only at this point we make an approximation and claim that $\mathbb F$ is small enough to state

$$\ln\left(\mathbb{I} - \mathbb{G}_{sp}\mathbb{F}\right) \approx -\mathbb{G}_{sp}\mathbb{F} - \frac{1}{2}\mathbb{G}_{sp}\mathbb{F}\mathbb{G}_{sp}\mathbb{F}$$
(12.101)

We neglect the terms from $(\mathbb{G}_{sp}\mathbb{F})^3$ and higher in orders of \mathbb{F} . We get

$$\mathcal{Z}_{q} = \mathcal{Z}_{sp} \int \mathcal{D}\bar{\phi}_{\mathbf{q},m} \mathcal{D}\phi_{\mathbf{q},m} \exp\left\{\frac{\sqrt{\beta V}}{g} \left(\Delta^{*}\phi_{\mathbf{0},m} + \Delta\bar{\phi}_{\mathbf{0},m}\right) - \operatorname{Tr}\left[\mathbb{G}_{sp}\mathbb{F}\right] + \sum_{\mathbf{q},m} \frac{\bar{\phi}_{\mathbf{q},m}\phi_{\mathbf{q},m}}{g} - \frac{1}{2}\operatorname{Tr}\left[\mathbb{G}_{sp}\mathbb{F}\mathbb{G}_{sp}\mathbb{F}\right]\right\}.$$
(12.102)

What about the terms linear in the fluctuation fields? They have to vanish! If we correctly determined the saddle point, then that means that the derivative (i.e. small derivations) vanishes. This then results in:

$$\mathcal{Z}_{q} = \mathcal{Z}_{sp} \int \mathcal{D}\bar{\phi}_{\mathbf{q},m} \mathcal{D}\phi_{\mathbf{q},m} \exp\left\{\sum_{\mathbf{q},m} \frac{\bar{\phi}_{\mathbf{q},m}\phi_{\mathbf{q},m}}{g} - \frac{1}{2}\operatorname{Tr}\left[\mathbb{G}_{sp}\mathbb{F}\mathbb{G}_{sp}\mathbb{F}\right]\right\} \quad (12.103)$$

and so the quantity that we need to calculate is $\operatorname{Tr} [\mathbb{G}_{sp} \mathbb{F} \mathbb{G}_{sp} \mathbb{F}]$. The remaining path integral will be denoted by \mathcal{Z}_{fl} , the partition sum of fluctuations, so that $\mathcal{Z}_q = \mathcal{Z}_{sp} \mathcal{Z}_{fl}$.

12.8.2 Gaussian fluctuations

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In the first term the sum runs over positive and negative ${\bf q}$ but this can be symmetrized through

$$\sum_{\mathbf{q},m} \frac{\phi_{\mathbf{q},m}\phi_{\mathbf{q},m}}{g} = \frac{1}{2} \sum_{\mathbf{q},m} \frac{1}{g} \left(\bar{\phi}_{-\mathbf{q},-m}\phi_{-\mathbf{q},-m} + \bar{\phi}_{\mathbf{q},m}\phi_{\mathbf{q},m} \right)$$
$$= \frac{1}{2} \sum_{\mathbf{q},m} \left(\begin{array}{c} \bar{\phi}_{\mathbf{q},m} & \phi_{-\mathbf{q},-m} \end{array} \right) \cdot \frac{1}{g} \left(\begin{array}{c} 1 & 0 \\ 0 & 1 \end{array} \right) \cdot \left(\begin{array}{c} \phi_{\mathbf{q},m} \\ \bar{\phi}_{-\mathbf{q},-m} \end{array} \right).$$
(12.104)

Using this result, performing the matrix multiplications, and taking the trace, we we can write the partition sum in the following "Gaussian integral" form

$$\mathcal{Z}_{fl} = \int \mathcal{D}\bar{\phi}_{\mathbf{q},m} \mathcal{D}\phi_{\mathbf{q},m} \exp\left\{-\frac{1}{2}\sum_{\mathbf{q},m} \left(\begin{array}{c} \bar{\phi}_{\mathbf{q},m} & \phi_{-\mathbf{q},-m} \end{array} \right), \quad (12.105) \\ \cdot \left(\begin{array}{c} M_{11}(\mathbf{q},i\varpi_m) & M_{12}(\mathbf{q},i\varpi_m) \\ M_{21}(\mathbf{q},i\varpi_m) & M_{22}(\mathbf{q},i\varpi_m) \end{array} \right) \cdot \left(\begin{array}{c} \phi_{\mathbf{q},m} \\ \bar{\phi}_{-\mathbf{q},-m} \end{array} \right) \right\} (12.106)$$

where

$$M_{11}(\mathbf{q}, i\varpi_m)$$
(12.107)
= $\frac{1}{\beta V} \sum_{\mathbf{k}, n} \frac{(i\nu_{m+n} + \xi_{\mathbf{q}+\mathbf{k}})}{(i\nu_{m+n} + E_{\mathbf{q}+\mathbf{k}})(i\nu_{m+n} - E_{\mathbf{q}+\mathbf{k}})} \frac{(i\nu_n - \xi_{\mathbf{k}})}{(i\nu_n + E_{\mathbf{k}})(i\nu_n - E_{\mathbf{k}})} - \frac{1}{g}$

and

$$M_{22}(\mathbf{q}, i\varpi_m)$$
(12.108)
= $\frac{1}{\beta V} \sum_{\mathbf{k}, n} \frac{(i\nu_{m+n} - \xi_{\mathbf{q}+\mathbf{k}})}{(i\nu_{m+n} + E_{\mathbf{q}+\mathbf{k}})(i\nu_{m+n} - E_{\mathbf{q}+\mathbf{k}})} \frac{(i\nu_n + \xi_{\mathbf{k}})}{(i\nu_n + E_{\mathbf{k}})(i\nu_n - E_{\mathbf{k}})} - \frac{1}{g}$

and

$$M_{12}(\mathbf{q}, i\varpi_m) = \frac{1}{\beta V} \sum_{\mathbf{k}, n} \frac{\Delta^2}{(i\nu_{m+n} + E_{\mathbf{q}+\mathbf{k}}) (i\nu_{m+n} - E_{\mathbf{q}+\mathbf{k}}) (i\nu_n + E_{\mathbf{k}}) (i\nu_n - E_{\mathbf{k}})}$$
(12.109)
$$M_{21}(\mathbf{q}, i\varpi_m) = \frac{1}{\beta V} \sum \frac{(\Delta^*)^2}{(i\nu_{m+n} + E_{\mathbf{q}+\mathbf{k}}) (i\nu_{m+n} - E_{\mathbf{q}+\mathbf{k}}) (i\nu_{m+n} - E_{\mathbf{k}})}$$

$$M_{21}(\mathbf{q}, i\varpi_m) = \frac{1}{\beta V} \sum_{\mathbf{k}, n} \frac{(\Delta)}{(i\nu_{m+n} + E_{\mathbf{q}+\mathbf{k}}) (i\nu_{m+n} - E_{\mathbf{q}+\mathbf{k}}) (i\nu_n + E_{\mathbf{k}}) (i\nu_n - E_{\mathbf{k}})}$$
(12.110)

You will have noticed that we let the matrix elements depend on the bosonic Matsubara frequencies $i\varpi_m = i(2\pi m/\beta)$. If we remember our short hand notations

$$i\nu_{m+n} = i\varpi_m + i\omega_n + \zeta \tag{12.111}$$

$$i\nu_n = i\omega_n + \zeta \tag{12.112}$$

then it is clear where these appear. The matrix \mathbb{M} is at the heart of our treatment of the fluctuations! It acts like a bosonic Green's function for the pair fields. It has some symmetry properties which can be derived from (12.107)–(??) by shifting the summation variables. We find

$$M_{11}(\mathbf{q}, i\varpi_m) = M_{22}(-\mathbf{q}, -i\varpi_m).$$
(12.113)

Moreover, since our saddle-point result shows us that $|\Delta|$ is fixed by the gap equation but we can choose the phase independently, we put Δ real and get

$$M_{12}(\mathbf{q}, i\varpi_m) = M_{21}(\mathbf{q}, i\varpi_m) = M_{21}(-\mathbf{q}, -i\varpi_m) = M_{12}(-\mathbf{q}, -i\varpi_m).$$
(12.114)

We still need to take sums over fermionic Matsubara frequencies, and integrals over \mathbf{k} in the matrix elements, this will be a bundle of joy for those who love complex analysis and residue calculus. More generally, we will have to study the poles of the components $M_{ij}(\mathbf{q}, z)$ in the complex plane to find excitations: poles in the Green's functions give us the quasiparticle spectrum!

12.8.3 Fluctuation free energy

The bosonic path integral is easier than the fermionic one, since we don't have to worry about the signs. We do have to worry not to double-count the fields. Since we sum over all \mathbf{q} , and seeing the symmetry properties of \mathbb{M} , each term appears twice. We can restrict ourselves to half the \mathbf{q}, m space and still get all the terms:

$$\frac{1}{2} \sum_{\mathbf{q},m} \left(\begin{array}{c} \bar{\phi}_{\mathbf{q},m} & \phi_{-\mathbf{q},-m} \end{array} \right) \cdot \mathbb{M}(\mathbf{q},i\varpi_m) \cdot \left(\begin{array}{c} \phi_{\mathbf{q},m} \\ \bar{\phi}_{-\mathbf{q},-m} \end{array} \right)$$
$$= \sum_{\substack{\mathbf{q},m \\ q_z \ge 0}} \left(\begin{array}{c} \bar{\phi}_{\mathbf{q},m} & \phi_{-\mathbf{q},-m} \end{array} \right) \cdot \mathbb{M}(\mathbf{q},i\varpi_m) \cdot \left(\begin{array}{c} \phi_{\mathbf{q},m} \\ \bar{\phi}_{-\mathbf{q},-m} \end{array} \right).$$

Similarly,

$$\begin{split} \int & \mathcal{D}\bar{\phi}_{\mathbf{q},m} \mathcal{D}\phi_{\mathbf{q},m} = \prod_{\mathbf{q},m} \int d\bar{\phi}_{\mathbf{q},m} d\phi_{\mathbf{q},m} \\ &= \prod_{\substack{\mathbf{q},m \\ q_z \ge 0}} \int d\bar{\phi}_{\mathbf{q},m} d\phi_{\mathbf{q},m} \int d\bar{\phi}_{-\mathbf{q},-m} d\phi_{-\mathbf{q},-m}. \end{split}$$

Therefore, when we integrate

$$\mathcal{Z}_{fl} = \int \mathcal{D}\bar{\phi}_{\mathbf{q},m} \mathcal{D}\phi_{\mathbf{q},m} \exp\left\{\frac{1}{2} \sum_{\mathbf{q},m} \left(\begin{array}{c} \bar{\phi}_{\mathbf{q},m} & \phi_{-\mathbf{q},-m} \end{array} \right) \cdot \mathbb{M}(\mathbf{q},i\varpi_m) \cdot \left(\begin{array}{c} \phi_{\mathbf{q},m} \\ \bar{\phi}_{-\mathbf{q},-m} \end{array} \right) \right\}$$

we get

$$\mathcal{Z}_{fl} = \prod_{\substack{\mathbf{q},m\\q_z \ge 0}} \frac{\pi^4}{\|\mathbb{M}(\mathbf{q}, i\varpi_m)\|},\tag{12.115}$$

with

$$\|\mathbb{M}(\mathbf{q}, i\varpi_m)\| = M_{11}(\mathbf{q}, i\varpi_m)M_{22}(\mathbf{q}, i\varpi_m) - M_{12}(\mathbf{q}, i\varpi_m)M_{21}(\mathbf{q}, i\varpi_m)$$

= $\Gamma(\mathbf{q}, i\varpi_m).$ (12.116)

This can be rewritten as

$$\mathcal{Z}_{fl} = \exp\left\{\sum_{\mathbf{q},m,(q_z \ge 0)} \ln\left[\frac{\pi^4}{\Gamma(\mathbf{q},i\varpi_m)}\right]\right\} = \exp\left\{\frac{1}{2}\sum_{\mathbf{q},m} \ln\left[\frac{\pi^4}{\Gamma(\mathbf{q},i\varpi_m)}\right]\right\}.$$
(12.117)

The π^4 , unlike the minus sign we had before, gives an irrelevant factor for the bosons, shifting the overall free energy by a constant amount. We obtain

$$\mathcal{Z}_{fl} \propto \exp\left\{-\frac{1}{2}\sum_{\mathbf{q},m} \ln\left[\Gamma(\mathbf{q},i\varpi_m)\right]\right\}.$$
 (12.118)

The total thermodynamic potential per unit volume Ω can now be divided in a saddle-point contribution Ω_{sp} and a fluctuation contribution Ω_{fl} : the latter satisfies

$$\mathcal{Z}_{fl} = \exp\left\{-\beta V \Omega_{fl}\right\} \tag{12.119}$$

and since $\mathcal{Z} = \mathcal{Z}_{sp} \mathcal{Z}_{sp}$ leads to $\Omega = \Omega_{sp} + \Omega_{fl}$ we find

$$\Omega_{fl} = \frac{1}{2\beta V} \sum_{\mathbf{q},m} \ln \left[\Gamma(\mathbf{q}, i\varpi_m) \right]$$
with $\Gamma(\mathbf{q}, i\varpi_m) = M_{11}(\mathbf{q}, i\varpi_m) M_{11}(-\mathbf{q}, -i\varpi_m) - M_{12}^2(\mathbf{q}, i\varpi_m)$
(12.120)

where we used the symmetry properties of the fluctuation matrix (12.113) and (12.114).

The equations determining our system become the following. For the gap equation we still have the saddle-point condition:

$$\frac{\partial \Omega_{sp}(T,\mu,\zeta;\Delta)}{\partial \Delta}\Big|_{T,\mu,\zeta} = 0 \quad \longrightarrow \quad \Delta(T,\mu,\zeta),$$

but we have to insert this in the full thermodynamic potential (including fluctuations) $\Omega(T, \mu, \zeta; \Delta(T, \mu, \zeta)) = \Omega(T, \mu, \zeta)$ to apply thermodynamic relations! For example, the number equations are given by the thermodynamic relations

$$n = -\left. \frac{\partial \Omega(T, \mu, \zeta)}{\partial \mu} \right|_{T, \zeta} \tag{12.121}$$

$$\delta n = - \left. \frac{\partial \Omega(T, \mu, \zeta)}{\partial \zeta} \right|_{T, \mu} \tag{12.122}$$

and for the density difference $\delta n = \delta n_{sp} + \delta n_{fl}$ we just derive to ζ keeping μ constant. Now remember our previous discussion: when we keep the Δ as a variable we have

$$n = -\left. \frac{\partial \Omega\left[T, \mu, \zeta; \Delta\right]}{\partial \mu} \right|_{T,\zeta,\Delta} - \left. \frac{\partial \Omega\left[T, \mu, \zeta; \Delta\right]}{\partial \Delta} \right|_{T,\zeta,\mu} \times \left. \frac{\partial \Delta(T, \mu, \zeta)}{\partial \mu} \right|_{T,\zeta}.$$
 (12.123)

Only $\partial \Omega_{sp}[T, \mu, \zeta; \Delta] / \partial \Delta$ will vanish: the partial derivative of Ω_{fl} will remain! So we get

$$n = -\left. \frac{\partial \Omega\left[T, \mu, \zeta; \Delta\right]}{\partial \mu} \right|_{T,\zeta,\Delta} - \left. \frac{\partial \Omega_{fl}\left[T, \mu, \zeta; \Delta\right]}{\partial \Delta} \right|_{T,\zeta,\mu} \times \left. \frac{\partial \Delta(T, \mu, \zeta)}{\partial \mu} \right|_{T,\zeta} . \tag{12.124}$$

We can write this as a sum of saddle-point density and fluctuation density

$$n = n_{sp} + n_{fl}.$$
 (12.125)

with

$$\begin{cases} \left. n_{sp} = - \left. \frac{\partial \Omega_{sp} \left[T, \mu, \zeta; \Delta \right]}{\partial \mu} \right|_{T,\zeta,\Delta} \\ \left. n_{fl} = - \left. \frac{\partial \Omega_{fl} \left[T, \mu, \zeta; \Delta \right]}{\partial \mu} \right|_{T,\zeta,\Delta} - \left. \frac{\partial \Omega_{fl} \left[T, \mu, \zeta; \Delta \right]}{\partial \Delta} \right|_{T,\zeta,\mu} \times \left. \frac{\partial \Delta(T, \mu, \zeta)}{\partial \mu} \right|_{T,\zeta} \\ (12.126) \end{cases}$$

12.9 Summary

At this point, we can summarize the full set of equations for the problem, including fluctuations. As a function of temperature $T \ (= 1/(k_B\beta))$, chemical potentials μ, ζ and gap Δ , the thermodynamic potential per unit volume is given by

$$\Omega(T,\mu,\zeta;\Delta) = \Omega_{sp}(T,\mu,\zeta;\Delta) + \Omega_{fl}(T,\mu,\zeta;\Delta)$$
(12.127)



Figure 12.6: This figure illustrates the importance of including fluctuations. Nearly nowhere is this more evident than in the case of a two-dimensional Fermi gas (see [?]). Without taking into account fluctuations, the saddle point result predicts pairing in the 2D Fermi gas at T^* . Including fluctuations, this temperature is reduced to T_p . But the mere presence of pairing is still insufficient to guarantee superfluidity. Indeed, superfluidity is further suppressed by phase fluctuations and occurs only below T_{BKT} , the Berezinski-Kosterlitz-Thouless temperature.

where the saddle-point and quadratic fluctuation contributions are

$$\Omega_{sp}(T,\mu,\zeta;\Delta) = -\frac{1}{g} |\Delta|^2 - \frac{1}{\beta V} \sum_{\mathbf{k},n} \ln\left[-\left(i\nu_n + E_{\mathbf{k}}\right)\left(i\nu_n - E_{\mathbf{k}}\right)\right], \quad (12.128)$$
$$\Omega_{fl}(T,\mu,\zeta;\Delta) = \frac{1}{2\beta V} \sum_{\mathbf{q},m} \ln\left[M_{11}(\mathbf{q},i\varpi_m)M_{11}(-\mathbf{q},-i\varpi_m) - M_{12}^2(\mathbf{q},i\varpi_m)\right]. \quad (12.129)$$

Here the fluctuation matrix elements are

$$M_{11}(\mathbf{q}, i\varpi_m) = \frac{1}{\beta V} \sum_{\mathbf{k}, n} \frac{\left(i\nu_{m+n} + \xi_{\mathbf{q}+\mathbf{k}}\right)}{\left(i\nu_{m+n} + E_{\mathbf{q}+\mathbf{k}}\right)\left(i\nu_{m+n} - E_{\mathbf{q}+\mathbf{k}}\right)} \frac{\left(i\nu_n - \xi_{\mathbf{k}}\right)}{\left(i\nu_n + E_{\mathbf{k}}\right)\left(i\nu_n - E_{\mathbf{k}}\right)} - \frac{1}{g}$$
(12.130)
$$M_{11}(\mathbf{q}, i\varpi_m) = \frac{1}{2} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n + E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\omega_n - E_{\mathbf{k}}\right)\left(i\omega_n - E_{\mathbf{k}}\right)} - \frac{1}{g} \sum_{\mathbf{k}, n} \frac{\Delta^$$

$$M_{12}(\mathbf{q}, i\varpi_m) = \frac{1}{\beta V} \sum_{\mathbf{k}, n} \frac{\Delta^2}{\left(i\nu_{m+n} + E_{\mathbf{q}+\mathbf{k}}\right) \left(i\nu_{m+n} - E_{\mathbf{q}+\mathbf{k}}\right) \left(i\nu_n + E_{\mathbf{k}}\right) \left(i\nu_n - E_{\mathbf{k}}\right)}$$
(12.131)

In these expressions

$$i\nu_n = i\omega_n + \zeta = i(2n+1)\pi/\beta + \zeta \tag{12.132}$$

are the shifted fermionic Matsubara frequencies and $\varpi_m = 2m\pi/\beta$ are the bosonic Matsubara frequencies. Furthermore, $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}$ is the Bogoliubov dispersion with $\xi_{\mathbf{k}} = k^2 - \mu$. Note that the Matsubara summations in the matrix elements can be performed, simplifying the results so that only a **k**-integral is left. The fermionic Matsubara summation in M_{11} results in

$$M_{11}(\mathbf{q}, i\varpi_m) = -\frac{1}{g} + \frac{1}{V} \sum_{\mathbf{k}} \frac{\sinh(\beta E_{\mathbf{k}})}{\cosh(\beta E_{\mathbf{k}}) + \cosh(\beta \zeta)} \frac{1}{2E_{\mathbf{k}}}$$
$$\times \left(\frac{(i\varpi_m + \xi_{\mathbf{q}+\mathbf{k}} - E_{\mathbf{k}}) (E_{\mathbf{k}} + \xi_{\mathbf{k}})}{(i\varpi_m + E_{\mathbf{q}+\mathbf{k}} - E_{\mathbf{k}}) (i\varpi_m - E_{\mathbf{q}+\mathbf{k}} - E_{\mathbf{k}})} - \frac{(i\varpi_m + E_{\mathbf{k}} + \xi_{\mathbf{q}+\mathbf{k}}) (E_{\mathbf{k}} - \xi_{\mathbf{k}})}{(i\varpi_m + E_{\mathbf{k}} + E_{\mathbf{q}+\mathbf{k}}) (i\varpi_m + E_{\mathbf{k}} - E_{\mathbf{q}+\mathbf{k}})} \right).$$
(12.133)

The fermionic Matsubara summation in M_{12} results in

$$M_{12}(\mathbf{q}, i\varpi_m) = -\frac{\Delta^2}{V} \sum_{\mathbf{k}} \frac{\sinh(\beta E_{\mathbf{k}})}{\cosh(\beta E_{\mathbf{k}}) + \cosh(\beta \zeta)} \frac{1}{2E_{\mathbf{k}}} \\ \times \left(\frac{1}{(i\varpi_m + E_{\mathbf{q}+\mathbf{k}} - E_{\mathbf{k}})(i\varpi_m - E_{\mathbf{q}+\mathbf{k}} - E_{\mathbf{k}})} + \frac{1}{(i\varpi_m + E_{\mathbf{q}+\mathbf{k}} + E_{\mathbf{k}})(i\varpi_m - E_{\mathbf{q}+\mathbf{k}} + E_{\mathbf{k}})} \right).$$
(12.134)

12.9. SUMMARY

The above equations provide the necessary ingredients to calculate the free energy, which in turn gives access to the thermodynamic variables of the system. Analyzing competing minima or evolving minima in the free energy also allows to derive phase diagrams for the system. In particular, from the saddle-point free energy (12.128) we derive the gap equation (the saddle-point condition):

$$\frac{\partial\Omega_{sp}(T,\mu,\zeta;\Delta)}{\partial\Delta}\Big|_{T,\mu,\zeta} = 0$$
(12.135)

from which we can extract $\Delta(T, \mu, \zeta)$, and the number equations

$$n = -\frac{\partial\Omega[T,\mu,\zeta;\Delta]}{\partial\mu}\Big|_{T,\zeta,\Delta} - \frac{\partial\Omega_{fl}[T,\mu,\zeta;\Delta]}{\partial\Delta}\Big|_{T,\zeta,\mu}\frac{\partial\Delta(T,\mu,\zeta)}{\partial\mu}\Big|_{T,\zeta} (12.136)$$

$$\delta n = -\frac{\partial\Omega[T,\mu,\zeta;\Delta]}{\partial\zeta}\Big|_{T,\mu,\Delta} - \frac{\partial\Omega_{fl}[T,\mu,\zeta;\Delta]}{\partial\Delta}\Big|_{T,\zeta,\mu}\frac{\partial\Delta(T,\mu,\zeta)}{\partial\zeta}\Big|_{T,\mu}. (12.137)$$

The gap and two number equations have to be fulfilled simultaneously, and need to be solved together to determine Δ, μ, ζ from $T, n, \delta n$.

The different approaches to the fermionic superfluidity can be catalogued through the gap and number equations that they consider. The full set, shown here, corresponds to the so-called "Gaussian pair fluctuation" (GPF) approach advocated by Hu, Liu and Drummond⁴. If the last terms in the number equations are dropped, we obtain the famous Nozières and Schmitt-Rink results⁵, ported to the path integral formalism by Sá de Melo, Randeria and Engelbrecht⁶. Finally, if also the fluctuation part Ω_{fl} is disregarded, we simply have the mean-field or saddle-point results discussed earlier. The results that we summarized here form the starting point of many currently on-going investigations: the effects of imbalance, the effects of reducing the dimensionality (to study the Berezinski-Kosterlitz-Thouless transitions⁷) and of optical potentials, the search for the Fulde-Ferrell-Larkin-Ovchinnikov state and other exotic pairing states. I hope that this (rather detailed) example shows you how quantum field theory is applied in practice in current, on-going research.

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⁶C.A.R. Sá de Melo, M. Randeria, and J. R. Engelbrecht, Phys. Rev. Lett. **71**, 3202 (1993).

⁷J. Tempere, S. Klimin, J.T. Devreese, Phys. Rev. A **79**, 053637 (2009); S.N. Klimin, J. Tempere, Jeroen P.A. Devreese, J. Low Temp. Phys. **165**, 261 (2011).

Appendix A

Functional derivatives

This part is not required for the course, but is helpful. Or confusing. Hopefully in the useful order.

Remember that the action S is a functional: it takes a function $\varphi(x)$ as input and spits out a real or complex number $S[\varphi(x)]$ ("operators" are different in that they take a function as input but return a function as well). We'll often need to figure out how the number changes as we change the input function,

$$\delta S = S[\varphi(x) + \delta\varphi(x)] - S[\varphi(x)] \tag{A.1}$$

Here δS is a number too, and it is linked to a very given way $\delta \varphi$ of disturbing the field φ . We can look at very specific "localized" disturbances and wonder for every point x how the value of the functional changes as we disturb the field at that point. This is called the functional derivative (or Fréchet derivative), and it is defined for a general functional $F[\varphi]$ as

$$\frac{\delta F}{\delta \varphi(y)} = \lim_{\varepsilon \to 0} \frac{F\left[\varphi(x) + \varepsilon \delta(x - y)\right] - F[\varphi(x)]}{\varepsilon}.$$
 (A.2)

What does this mean? First, note that $\delta F/\delta \varphi(y)$ itself is a *function* (of y), not a number, nor a functional¹. We've taken the input of the functional F, and added to this a small $(\varepsilon \to 0)$ disturbance $\delta(x - y)$ localized in y. The change in F due to this very specific disturbance determines the functional derivative.

We can use the functional derivative to calculate the change δF resulting from any disturbance $\delta \varphi(x)$:

$$\delta F = \int dx \, \frac{\delta F}{\delta \varphi(x)} \delta \varphi(x). \tag{A.3}$$

This implies that the total change in F upon variation of the function $\varphi(x)$ is a linear superposition of local changes, summed over the whole range of x

¹So, "taking the functional derivative" of F in $\varphi(y)$ is an operator: it takes the function $\varphi(y)$ and produces the function $\delta F/\delta\varphi(y)$. What function you get depends on which field realization you vary around.

values. It is clear that when we plug in $\delta\varphi(x) = \varepsilon\delta(x-y)$ we obtain the original definition again, so we could also use (A.3) as the defining relation of the functional derivative.

In practice, most of the time you will encounter one of a limited number of specific examples of functional derivatives. The main types of functional that we need are:

• Powers of a field:

$$S[\varphi(x)] = \int \varphi^n(x) dx \tag{A.4}$$

Applying the definition (A.2) we get

$$\frac{\delta S}{\delta \varphi(y)} = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left(\int \left(\varphi(x) + \varepsilon \delta(x - y) \right)^n dx - \int \varphi^n(x) dx \right)$$
$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left(\int n \varphi^{n-1}(x) \varepsilon \delta(x - y) dx + \mathcal{O}(\varepsilon^2) \right)$$
(A.5)

We used Newtons binomium for the $(a+b)^n$ integrand here. Now it's easy to perform the remaining integral, using the delta function:

$$\frac{\delta S}{\delta \varphi(y)} = n\varphi^{n-1}(y) \tag{A.6}$$

• Powers of the derivative of a field

$$S[\varphi(x)] = \int \left(\frac{d\varphi}{dx}\right)^n dx \tag{A.7}$$

That's a bit harder, as we need to formally keep $d\delta(x-y)/dx$ together,

$$\frac{\delta S}{\delta \varphi(y)} = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\int \left(\frac{d\varphi}{dx} + \varepsilon \frac{d\delta(x-y)}{dx} \right)^n dx - \int \varphi^n(x) dx \right]$$
$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\int n \left(\frac{d\varphi}{dx} \right)^{n-1} \varepsilon \frac{d\delta(x-y)}{dx} dx + \mathcal{O}(\varepsilon^2) \right]$$
(A.8)

before we get rid of it through integration by parts,

$$\frac{\delta S}{\delta \varphi(y)} = -\int n \frac{d}{dx} \left(\frac{d\varphi}{dx}\right)^{n-1} \delta(x-y) dx \tag{A.9}$$

and we obtain

$$\frac{\delta S}{\delta \varphi(y)} = -\left. n \frac{d}{dx} \left(\frac{d\varphi}{dx} \right)^{n-1} \right|_{x=y} \tag{A.10}$$

In particular, we often encounter n = 2 for which

$$n = 2 : \frac{\delta S}{\delta \varphi(y)} = -2 \left. \frac{d^2 \varphi}{dx^2} \right|_{x=y}$$

The subscript means that we have the evaluate the second derivative of the field in the point y.

• Linear kernels

$$S_{z}[\varphi(x)] = \int K(z, x)\varphi(x)dx \qquad (A.11)$$

are straightforward,

$$\frac{\delta S_z}{\delta \varphi(y)} = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int K(z, x) \left[\varphi(x) + \varepsilon \delta(x - y) - \varphi(x) \right] dx$$

$$\Rightarrow \frac{\delta S_z}{\delta \varphi(y)} = K(z, y)$$
(A.12)

Note that now the functional depends on a parameter z.

• The trivial functional

$$F_z[\varphi(x)] = \varphi(z) \tag{A.13}$$

just plucks the value of the field at a given point z, and doesn't care about the field anywhere else. It's functional derivative is

$$\frac{\delta F_z}{\delta \varphi(y)} = \delta(y - z) \tag{A.14}$$

When life gets tough, you can always revert to discretization to try to find an answer, for example

$$S[\varphi(x)] = \int f(\varphi(x))dx$$

$$\rightarrow \quad S[\varphi_0, \varphi_1, \dots, \varphi_N] = \sum_{j=0}^N f(\varphi_j)\Delta x_j \quad (A.15)$$

Note that if we have derivatives of the field, the way in which we discretize these derivatives will matter! That why in this example I just have a function of the field, I do not want to open Pandora's box in this appendix.

If you discretize the field $\varphi(x)$ in your mind, going back to the string of mass points with springs between them that we used as example in the chapter on classical Lagrangian field theory, it is clear that by a localized disturbance we mean wiggling a single mass point of the string and seeing how this affects functionals such as the action. Let's say we wiggle the mass point at y, so we have

$$\varphi(x) + \varepsilon \delta(x - y) \to \{\varphi_0, \varphi_1 \dots, \varphi_y + \varepsilon, \dots, \varphi_N\}$$
 (A.16)

The discretized action changes by

$$\delta S = \sum_{j} \delta_{j,y} \left[f(\varphi_j + \varepsilon) - f(\varphi_j) \right] \Delta x_j \tag{A.17}$$

where $\delta_{j.y}$ is the kronecker delta that selects the right point to tap. For small ε is this

$$\delta S = \varepsilon \sum_{j} \delta_{j,y} f'(\varphi_j) \Delta x_j \tag{A.18}$$

Now we can go back to the continuum limit

$$\delta S = \varepsilon \int \delta(x - y) f'(\varphi(x)) dx \tag{A.19}$$

So we get

$$S[\varphi(x)] = \int f(\varphi(x))dx \Rightarrow \frac{\delta S}{\delta\varphi(y)} = f'(\varphi(y))$$
(A.20)

Applying this to $f(x) = x^n$ we get the same result as in (A.6).

Finally, for

$$S[\varphi(x)] = \int \mathcal{L}(\varphi, \partial_{\mu}\varphi) dx, \qquad (A.21)$$

comparing

$$\delta S = \int \left(\frac{\partial \mathcal{L}}{\partial \varphi} - \partial_{\mu} \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi)}\right) \delta \varphi dx.$$
 (A.22)

to (A.3) shows that

$$\frac{\delta S}{\delta \varphi} = \frac{\partial \mathcal{L}}{\partial \varphi} - \partial_{\mu} \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \varphi)}.$$
 (A.23)

Stating that the variation of the action is zero for any small change around the classical field in the field, is equivalent to stating that the functional derivative of the action, evaluated in the classical field, is zero.