Concepts of Many-Body Physics

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Contents

These lecture notes serve as accompaniment to the Master's course Statistical Physics and Condensed Matter Theory 1 given at the University of Amsterdam. Many parts are directly derived from the book "Condensed Matter Field Theory" by A. Altland and B. Simons, their notation being closely followed in many instances; the equation labels "CMFT(#.#)" in the margins directly refer to equation numbering in this book, which should anyway be consulted for a more complete coverage of the field.

Introduction

The great adventure that is physics consists of three different but complementary quests. The starting point is surely the cataloguing of all fundamental constituents of matter. As far as everyday life is concerned, the most important of these are atomic nuclei, electrons and photons. This list is however not exhaustive. For example, we know that nuclei are in fact composite objects made of protons and neutrons. In turn, these are composites of quarks. Whether this chain of ascendency ever terminates remains a quite inspirational mystery. In any case, our catalogue of fundamental constituents is exhaustive enough for most practical applications.

Second comes the characterization of the basic interactions between these constituents. The list of fundamental forces currently stands at four: the gravitational force on the one hand, and the electromagnetic, weak and strong nuclear forces on the other. Again here the classification into four forces is not set in stone. Electromagnetic and weak nuclear forces are unified in electroweak theory; grand unified theory then attempts to also incorporate the strong nuclear force. Whether there are indeed only four forces, and whether these are in the end manifestations of a single all-encompassing force again remains a mystery. Nonetheless, as for fundamental constituents, we can be quite satisfied with our catalogue of fundamental forces.

The third quest is more subtle, but naturally emerges as one tries to blend fundamental constituents interacting with each other in larger and larger numbers. Put simply, one immediately faces a wall of complexity when one tries to translate detailed information about constituents and fundamental interactions into firm predictions for physical behaviour of many-body systems. The minimal illustration of this is obtained by considering (Newtonian) gravitationally-interacting spherically-symmetric bodies. The two-body case (Kepler problem) can be solved exactly, allowing to predict positions and velocities at any time (past or future) from a set of initial conditions. Strikingly, this feature of exact solvability is immediately lost (except for fine-tuned initial conditions) when the problem is complicated by the addition of more bodies. As shown by Bruns and Poincaré, there cannot be an analytical solution to the 3-body problem for arbitrary initial conditions. Motion is then not periodic in general, but rather chaotic. This is also the case for the n-body problem. If we cannot even solve such an already-oversimplified problem, what hope can we possibly have of predicting anything about systems of very (thermodynamically!) large numbers of different types of particles interacting with each other with all available forces? Can one understand barred spiral galaxies from Newtonian gravity? Is the crystal structure of piperidinium copper bromide $(C_5H_{12}N)_2CuBr_4$ somehow hidden in the Coulomb force?

Facing the cliff face of the many-body problem, the fatalistic researcher will either close up shop or refocus towards simply pushing the first two above-mentioned quests further. A more adventurous thinker will however view this third quest, which one usually refers to as the physics of *emergence*, as carrying more potential for astounding discoveries, and welcome every opportunity to 'add a bit more junk' as an additional chance of generating something unexpected. This contrast was perhaps best expressed by Primo Levi in his book 'Il sistema periodico', when he describes how the element zinc reacts differently to acid as a function of its level of purity:

'... l'elogio della purezza, che protegge dal male come un usbergo; l'elogio dell'impurezza, che dà adito ai mutamenti, cioè alla vita. Scartai la prima, disgustosamente moralistica, e mi attardai a considerare la seconda, che mi era piú congeniale.'[1] This more congenial path is the one followed by the modern many-body physicist, and is the one which I will do my best to expose in this book.

In fact, one can easily get carried away with optimism when thinking about the current state of physics. After all, looking at the world around us with the eyes of a knowledgeable physicist[2], one can sympathise with the statement from Laughlin and Pines [1] that almost every *thing* we are confronted with in daily life can be explained by simple nonrelativistic quantum mechanics based on the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle, \tag{1}$$

where $\hbar$ is Planck's constant. The Hamiltonian here describes N_e electrons of fundamental charge $-e$ and mass m, together with N_i atomic nuclei of mass M_α and charge $Z_\alpha e$ ($\alpha = 1, ..., N_i$), interacting following Coulomb's law:

$$H = \sum_j^{N_e}\frac{-\hbar^2}{2m}\boldsymbol{\nabla}_j^2 + \sum_\alpha^{N_i}\frac{-\hbar^2}{2M_\alpha}\boldsymbol{\nabla}_\alpha^2 - \sum_j^{N_e}\sum_\alpha^{N_i}\frac{Z_\alpha e^2}{|\boldsymbol{r}_j - \boldsymbol{R}_\alpha|} + \sum_{j<k}^{N_e}\frac{e^2}{|\boldsymbol{r}_j - \boldsymbol{r}_k|} + \sum_{\alpha<\beta}^{N_i}\frac{Z_\alpha Z_\beta e^2}{|\boldsymbol{R}_\alpha - \boldsymbol{R}_\beta|} \tag{2}$$

in which $\boldsymbol{r}_j$ is the spatial coordinate of electron j and $\boldsymbol{R}_\alpha$ that of ion α. Missing from this theory are of course any interactions associated to the nuclear forces, and gravity. We should also include spin, to be able to handle problems in magnetism. Coupling to light is easily included; we can even build in special relativity, we'd then simply call this whole edifice QED (quantum electrodynamics).

Without even going that far, reasonings based on (1, 2) give us an explanation of the sizes of atoms, the strength and scale of chemical bonds, basic properties of bulk matter such as sound waves, why certain materials conduct electricity while others don't, why some are transparent to light of certain frequencies and others not. The accuracy to which this 'Theory of Everything' thus describes basic physical properties and processes is simply astounding, and we can easily get ahead of ourselves and repeat the common mantra that it captures all the essential features for explaining essentially all that we see around us.

There exist however more complicated phenomena which we cannot reasonably expect to explain from our Theory of Everything. Basic life forms, the human brain, the nonsense of stock market fluctuations, even some very-typical-looking ceramics which happen to superconduct at relatively high temperature cannot be modelled in any practically feasible way starting from (1, 2). Besides our model itself being at best only distantly related to what we want to describe, the *rules* themselves are subject to being questioned. For example, many phenomena observed at the 'human' scale can be much better described starting from classical mechanics; it would then be at least less than economical, perhaps at most even nonsensical, to start from a microscopic quantum theory. Citing Laughlin and Pines again, 'So the triumph of the reductionism of the Greeks is a pyrrhic victory: We have succeeded in reducing all of ordinary physical behavior to a simple, correct Theory of Everything only to discover that it has revealed exactly nothing about many things of great importance.'

[1] '... the praise of purity, which protects from evil like a coat of mail; the praise of impurity, which gives rise to changes, in other words to life. I discarded the first, disgustingly moralistic, and I lingered to consider the second, which I found more congenial.'

[2] To qualify for this, you have to master classical and quantum mechanics, thermodynamics and statistical physics, electromagnetism and all the necessary mathematics (Fourier transforms, calculus, linear algebra, perhaps a bit of complex analysis), and ideally be at ease with a few more subsidiary subjects such as condensed matter physics...

In order to make progress, one has to make some sacrifices. First of all, perhaps not all degrees of freedom in (2) are relevant to a specific problem one might think about. For example, if we are interested in the motion of electrons in a conductor, we might reasonably assume that the nuclei are simply sitting at fixed positions and ignore their motion. Writing an effective model involving this reduced number of degrees of freedom then provides a more economical starting point.

Once a reasonable effective model has been written down, explicit calculations can be attempted. In most cases however, our solution capabilities fall far short of our desires. We might like to know what the frequency-dependent conductivity of the two-dimensional Hubbard model is as a function of interaction strength, filling and temperature, but getting there is no easy task. The dream of finding exact solutions to strongly-correlated many-body systems has only really been realized in the world of one-dimensional quantum (or equivalently, two-dimensional classical) physics, but these firmly-grounded results, though extremely instructive, do not extend to higher dimensions.

Over the last few decades, physicists have thus built extensive frameworks to handle such unsolvable problems as best as possible. In a first instance, perturbation theory is the natural starting point. The strategy is simple: from an exactly-solved simple base system (most commonly: a free (noninteracting) theory, all of whose correlation functions are readily computable), try to approach the desired system by systematically computing the effects of the perturbations required to bring you from the base system to the desired one. Clever tricks (for example: partial resummations to infinite order) have been devised to do this in a meaningful way, and this will be the subject of Chapter 5.

Another very important general approach has emerged, known as mean-field theory. Finding it's origins in the idea of the 'molecular field' of Pierre Weiss, modern-day mean-field theory is possibly the most commonly-applied tool to deal with an interacting many-body problem. The idea is to look for a replacement effective 'mean-field' model in which interactions are present, but not higher correlations. Whether such an effective mean-field theory makes sense for a given situation depends on many details, which shall be discussed in Chapter 6. Mean-field theory has been pushed and extended today to something one perhaps better labels as effective field theory; here, one can altogether do without a microscopic starting point, and guide oneself with simple symmetry considerations to write down a 'top-down' effective model for a given class of problems. The fundamental concept of importance here is that of *universality*, namely that the details of the microscopic starting point possess a certain degree of flexibility, by which we mean that the resulting low-energy physics is invariant under such microscopic modifications. This will also be discussed in Chapter 6.

Being able to handle a given theory must ultimately mean that we are in a position to answer questions relevant to experiments. There exist a large number of experimental probes for condensed-matter systems, and all require specific treatments. On the other hand, one can theoretically handle most cases formally as specializations of a general framework, response theory, which we will expose in its simplest form in Chapter 7.

The purpose of this book is to give its reader a basic, systematically organized grounding in the language and techniques of many-body physics, in both its classical and quantum manifestations, enabling not only the formulation of a proper underlying theory, but also the treatment of it up to the point where useful physical predictions can be obtained.

Chapter 1

Collective phenomena

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Interacting many-body systems come in very many shapes and forms, and to tell you the truth, there are few which we understand to any satisfying degree. For some however, we can claim to know more or less everything. It is natural to use the simplest of these as 'stepping stones' towards more elaborate cases; the purpose of this chapter is to introduce a prototypical simple model of coupled oscillators, and to hereby rehearse most of the basic physics needed to understand later chapters.

1.1 The classical harmonic chain

Starting from our theory of everything (eq:MBP:HNRSE (2)), let us concentrate on the core ions only, assuming that electrons have no dynamics and remain bound to their respective ion. Furthermore, we shall treat the atom's dynamics classically. We will also assume the simplest possible geometry, which is a one-dimensional chain. Without specifying the precise details, we expect the interatomic potential[1] to have some minimum at a characteristic distance a which naturally defines the lattice spacing of our chain.

If we were to remove all fluctuations by going to zero temperature, the system would be frozen in a configuration in which all the atoms sit precisely at the required lattice spacing, $R_I \equiv \bar{R}_I = Ia$ (here, we label positions with an integer index I, putting the origin of coordinates on the atom with label 0). Deviations from this configuration, induced by perturbations or thermal fluctuations, carry a price in kinetic and potential energy. The kinetic energy is still given by the free-particle term with momentum P_I. Since the interatomic potential is assumed to have a minimum at distance a, the energy is approximately quadratic in the small deviations from equilibrium. We can thus consider the reduced low-energy effective Hamiltonian (giving our atoms a mass m from now on)

$$H = \sum_{I=1}^{N} \left(\frac{P_I^2}{2m} + \frac{k_s}{2}(R_{I+1} - R_I - a)^2 \right). \tag{1.1}$$

CMFT(1.2)

As is immediately clear, this Hamiltonian is effectively that of N point-like particles connected by springs obeying Hooke's law, whose parameter k_s is taken as given (it's simply the second derivative of the effective interatomic potential, but the details of this don't need to be specified).

[1] A good example being a Lennard-Jones potential.

1.1.1 Lagrangian formulation

From (1.1), one could proceed directly and solve the equations of motion exactly. We could consider doing this in the Lagrangian formulation, in which case we consider

$$L = T - U = \sum_{I=1}^{N} \left(\frac{m}{2} \dot{R}_I^2 - \frac{k_s}{2} (R_{I+1} - R_I - a)^2 \right). \tag{1.2}$$

CMFT(1.2) CMFT(1.3)

Let us however push forward the idea of simplifying our problem as much as possible, while keeping the interesting physics on board. For large N, we can expect boundary effects to become negligible, at least as far as the bulk physical properties are concerned. We're free to impose *e.g.* the topology of a circle, using periodic boundary conditions $R_{N+1} = R_1$. We shall also consider the low-energy sector, assuming that only small deviations $|R_I(t) - \bar{R}_I| \ll a$ are present. Defining $R_I(t) = \bar{R}_I + \phi_I(t)$ with $\phi_{N+1}(t) = \phi_1(t)$, the Lagrangian becomes

$$L = \sum_{I=1}^{N} \left(\frac{m}{2} \dot{\phi}_I^2 - \frac{k_s}{2} (\phi_{I+1} - \phi_I)^2 \right). \tag{1.3}$$

CMFT(1.3a)

We can also use the fact that we're not interested in phenomena at the atomic scale, but only in macroscopic low-energy phenomena, for example the chain's bulk specific heat. This leads us to take a continuum limit, namely to ignore discreteness of the atomic spacing and describe the system by effective, continuous degrees of freedom. Such a description makes sense if relative fluctuations are weak, in other words if the displacement of a given atom is more or less equal to the displacement of its neighbours. We thus define a continuous function $\phi(x)$, which describes the displacement of the atom at position x. The correspondence can be written as

$$\begin{aligned} &\phi_I \to a^{1/2} \phi(x)|_{x=Ia}, \\ &\phi_{I+1} - \phi_I \to a^{1/2} (\phi(x+a) - \phi(x))|_{x=Ia} = a^{3/2} \partial_x \phi(x)|_{x=Ia} + \cdots \end{aligned} \tag{1.4}$$

in which $\cdots$ denotes higher derivative terms which we drop for the moment (they lead to anharmonicities). Note that with this convention, the function ϕ has dimensionality $[\phi(x,t)] = [\text{length}]^{1/2}$. Using the identity

$$\sum_{I=1}^{N} (...) \to \frac{1}{a} \int_0^L dx (...) \tag{1.5}$$

with $L = Na$, we can now write our Lagrangian in the continuum limit,

$$L[\phi] = \int_0^L dx \mathcal{L}(\phi, \partial_x \phi, \dot{\phi}), \qquad \mathcal{L}(\phi, \partial_x \phi, \dot{\phi}) = \frac{m}{2} \dot{\phi}^2 - \frac{k_s a^2}{2} (\partial_x \phi)^2. \tag{1.6}$$

CMFT(1.4)

$\mathcal{L}$ is the **Lagrangian density** with dimensionality [energy]/[length].

Finally, the classical action of our effective low-energy theory is given by

$$S[\phi] = \int dt L[\phi] = \int dt \int_0^L dx \mathcal{L}(\phi, \partial_x \phi, \dot{\phi}). \tag{1.7}$$

CMFT(1.5)

We have gone from an N-point particle description to one involving continuous degrees of freedom represented by a **classical field**. Its dynamics are specified by **functionals** L and S which are continuum versions of the Lagrangian and action.

Fields and functionals
A **field** is a mapping

$$\phi : M \mapsto T, \qquad z \mapsto \phi(z), \tag{1.8}$$

from a "base manifold" M to a "target" or "field manifold" T. In the current example, $M = [0, L] \times [0, t] \subset \mathbb{R}^2$ and $T = \mathbb{R}$.

A **functional** is a mapping from a field into real numbers,

$$S : \phi \mapsto S[\phi] \in \mathbb{R} \tag{1.9}$$

(note: argument of a functional is conventionally written in square brackets).

To get the actual behaviour of model as a function of time, we need **equations of motion**. What do they look like here for our continuous classical field? How to obtain them? The answer is a simple extension of the principles used in the classical mechanics of single particles, most beautifully expressed in Hamilton's extremum principle[2], which we here apply to an infinite number of degrees of freedom.

The idea is thus to require that the action of our system be stationary. For the field $\phi(x, t)$, we thus define a variation (which by convention is defined to vanish at the system's spatial boundaries)

$$\phi(x, t) \to \phi(x, t) + \epsilon\eta(x, t) \tag{1.10}$$

CMFT(1.7a)

and require stationarity of the action explicitly:

$$\begin{aligned} S[\phi + \epsilon\eta] - S[\phi] &= \int dt \int_0^L dx \left[\frac{m}{2}(\dot{\phi} + \epsilon\dot{\eta})^2 - \frac{k_s a^2}{2}(\partial_x\phi + \epsilon\partial_x\eta)^2 \right] - S[\phi] \\ &= \epsilon \int dt \int_0^L dx (m\dot{\phi}\dot{\eta} - k_s a^2 \partial_x\phi\partial_x\eta) + O(\epsilon^2) \\ &= -\epsilon \int dt \int_0^L dx (m\ddot{\phi} - k_s a^2 \partial_x^2\phi)\eta + \epsilon \int_0^L dx m\dot{\phi}\eta|_{t=0}^T - \epsilon \int dt k_s a^2 \partial_x\phi\eta|_{x=0}^L + O(\epsilon^2) \end{aligned} \tag{1.11}$$

so stationarity (namely, asking that the first-order term in the variation vanishes) yields

$$\lim_{\epsilon\to 0} \frac{1}{\epsilon}(S[\phi + \epsilon\eta] - S[\phi]) = -\int dt (m\ddot{\phi} - k_s a^2 \partial_x^2\phi)\eta = 0 \tag{1.12}$$

since by definition we take the variation to vanish at the boundaries of space and time. Since this must hold true for any smooth η satisfying these boundary conditions, we get a wave equation for the field:

$$(m\partial_t^2 - k_s a^2 \partial_x^2)\phi(x, t) = 0 \tag{1.13}$$

CMFT(1.8)

whose solutions have the general form

$$\phi(x, t) = \phi_+(x - vt) + \phi_-(x + vt), \qquad v = a\sqrt{k_s/m} \tag{1.14}$$

and $\phi_\pm$ are *arbitrary* smooth functions. The **elementary excitations** are thus lattice vibrations propagating as **sound waves** with constant velocity v. The important point here is that

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[2] See A.2 for a reminder of Hamiltonian and Lagrangian formulations of the classical mechanics of single particles.

these **collective excitations** have little to do with the microscopic constituents themselves, but emerge in great generality in any system with similar microscopics containing kinetic and interaction energies. For example, in an interacting electron gas, collective excitations known as *plasmon* modes involving large numbers of electrons appear and determine much of the low-energy physics. Experience shows that merely *identifying* which are the relevant excitations in a given system is one of the crucial steps in the solution of a condensed matter problem.

Functional analysis

Let's consider a simple one-dimensional base manifold and a given functional F. This functional is differentiable if

$$F[f+\epsilon g]-F[f]=\epsilon\cdot DF_f[g]+O(\epsilon^2) \tag{1.15}$$

where $DF_f[g]$ is a linear functional, ϵ is a small parameter and g is an arbitrary function. The differential is given by

$$DF_f[g]=\int dx\frac{\delta F[f]}{\delta f(x)}g(x). \tag{1.16}$$

CMFT(1.14)

in which the functional differential is defined as

$$\frac{\delta F[f(x)]}{\delta f(y)}\equiv\lim_{\epsilon\to 0}\frac{1}{\epsilon}(F[f(x)+\epsilon\delta(x-y)]-F[f(x)]). \tag{1.17}$$

CMFT(1.15)

This is best illustrated with simple examples. For the simple functional $F[f]=\int dxf(x)$, we have

$$\frac{\delta F[f]}{\delta f(y)}=\lim_{\epsilon\to 0}\frac{1}{\epsilon}(\int dx(f(x)+\epsilon\delta(x-y))-\int dxf(x))=\int dx\delta(x-y)=1. \tag{1.18}$$

A slightly more complicated case is to consider the functional $F_x[f]$ (where x is a parameter) defined as $F_x[f]=\int dyG(x,y)f(y)$. It's functional differential is

$$\begin{aligned}\frac{\delta F_x[f]}{\delta f(z)}&=\lim_{\epsilon\to 0}\frac{1}{\epsilon}(\int dyG(x,y)[f(y)+\epsilon\delta(y-z)]-\int dyG(x,y)f(y)\\&=\int dyG(x,y)\delta(y-z)=G(x,z).\end{aligned} \tag{1.19}$$

Other things familiar from differential and integral calculus also find their parallels in functional analysis. For example, the chain rule takes the form

$$\frac{\delta F[g[f]]}{\delta f(x)}=\int dy\frac{\delta F[g]}{\delta g(y)}|_{g=g[f]}\frac{\delta g(y)[f]}{\delta f(x)}. \tag{1.20}$$

A functional can also be approximated by a functional Taylor expansion:

$$F[f]=F[0]+\int dx_1\frac{\delta F[f]}{\delta f(x_1)}|_{f=0}f(x_1)+\frac{1}{2}\int dx_1dx_2\frac{\delta^2F[f]}{\delta f(x_2)\delta f(x_1)}|_{f=0}f(x_1)f(x_2)+... \tag{1.21}$$

What we have just done is an example of **functional analysis** (see Supporting block). It is worth taking a moment and generalizing our reasoning to an (almost) arbitrary case. A derivation of equations of motion is then obtained by applying the principle of least action to a

generic field theory. Usually, field theory functionals are of the form

$$S[\phi] = \int_M d^m x \mathcal{L}(\phi^i, \partial_\mu \phi^i) \tag{1.22}$$ CMFT(1.16)

in which we assumed that the base manifold M is parametrized by an m-dimensional coordinate vector $x = \{x_\mu\}$. Usually, $m = d + 1$ with x_0 a time-like coordinate.

Let us assume that the field manifold has dimensionality n, and denote our field coordinates as ϕ^i. What makes things simple is that all info about the action S is contained in the *function* $\mathcal{L}$. We can repeat the simple variational steps above to this generic case:

$$\begin{aligned} S[\phi + \epsilon\theta] - S[\phi] &= \int_M d^m x \left[\mathcal{L}(\phi + \epsilon\theta, \partial_\mu \phi + \epsilon \partial_\mu \theta) - \mathcal{L}(\phi, \partial_\mu \phi)\right] \\ &= \int_M d^m x \left[\frac{\partial \mathcal{L}}{\partial \phi^i}\theta^i + \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^i}\partial_\mu \theta^i\right]\epsilon + O(\epsilon^2) \\ = \int_M d^m x \left[\frac{\partial \mathcal{L}}{\partial \phi^i} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^i}\right]\theta^i \epsilon + \int_{\partial M} d^{m-1}\sigma_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^i}\theta^i \epsilon + O(\epsilon^2) & \end{aligned} \tag{1.23}$$

Here, ∂M is the boundary of the base manifold M, and σ_μ is the boundary integration element. We assume that the variation vanishes on boundary of base manifold, $\theta|_{\partial M} = 0$. The functional derivative is thus (using (1.16)) CMFT(1.14)

$$\frac{\delta S[\phi]}{\delta \phi^i(x)} = \frac{\partial \mathcal{L}}{\partial \phi^i(x)} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi^i(x))}. \tag{1.24}$$

The **stationarity of the functional** (1.22) CMFT(1.16) is thus equivalent to the set of functional equations

$$\frac{\partial \mathcal{L}}{\partial \phi^i(x)} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi^i(x))} = 0, \qquad \forall\, x, i \tag{1.25}$$ CMFT(1.17)

which are known as the **Euler-Lagrange equations** for field theory.

Comment: for $d = 0$ and $x_0 = t$, these reduce to the E-L equation of a point particle in n-dimensional space.

1.1.2 Hamiltonian formulation

Energy of sound waves ? Need Hamiltonian form, again generalizing from point particles to the continuum.

For a point particle: conjugate momentum defined from Lagrangian as $p \equiv \partial_{\dot{x}} L$.

For our ϕ_I variables in (1.3): CMFT(1.3a)

$$\pi_I = m\dot{\phi}_I \tag{1.26}$$

so

$$H = \sum_I \pi_I \dot{\phi}_I - L = \sum_I \left(\frac{\pi_I^2}{2m} + \frac{k_s}{2}(\phi_{I+1} - \phi_I)^2\right). \tag{1.27}$$

In the continuum, let us define the **canonical momentum** conjugate to ϕ from the Lagrangian density as

$$\pi(x) \equiv \frac{\partial \mathcal{L}(\phi, \partial_x \phi, \dot{\phi})}{\partial \dot{\phi}(x)}. \tag{1.28}$$ CMFT(1.9)

The **Hamiltonian density** is then defined as usual,

$$\mathcal{H}(\phi, \partial_x \phi, \pi) = (\pi \dot{\phi} - \mathcal{L}(\phi, \partial_x \phi, \dot{\phi}))|_{\dot{\phi}=\dot{\phi}(\phi,\pi)} \tag{1.29}$$ CMFT(1.10)

with the full Hamiltonian being $H = \int_0^L dx \mathcal{H}$.

We have $\pi(x,t) = m\dot{\phi}(x,t)$ and

$$H[\pi, \phi] = \int dx (\frac{\pi^2}{2m} + \frac{k_s a^2}{2} (\partial_x \phi)^2). \tag{1.30}$$ CMFT(1.11)

For *e.g.* a right-moving excitation, $\phi(x,t) = \phi_+(x - vt)$, we have $\pi(x,t) = m\partial_t \phi_+(x - vt) = -mv\partial_x \phi_+(x - vt)$ so $H[\pi, \phi] = mv^2 \int dx (\partial_x \phi(x - vt))^2 = mv^2 \int dx (\partial_x \phi(x))^2$ (by using periodic boundary conditions) which is a positive definite time-independent expression.

Comment on symmetry The notion of symmetry is extremely important in classical and quantum dynamics. Noether's theorem finds its way into field theory (see Supplement at the end of this Chapter). Here, let us simple make a few basic but fundamentally important observations.

For infinitely shallow excitation $\partial_x \phi_+ \to 0$, the energy vanishes.

$\to$**symmetry**: H invariant under uniform translation of all atoms, $\phi_I \to \phi_I + \delta$

Global translation does not affect internal energy. Real crystal: coordinates fixed, $R_I = Ia \to \phi_I = 0$. Translational symmetry is **spontaneously broken**, the solid decides where it wants to rest.

Remnant of this symmetry: infinite-wavelength (low-energy) deviations from ground state with broken symmetry cost a vanishingly small amount of energy.

So: **symmetry** $\to$low-energy excitations (further discussed in CMFT Chap. 6).

Some physics: specific heat of classical harmonic chain From statistical mechanics: energy density

$$u = \frac{1}{L} < H >= -\frac{1}{L} \partial_\beta \ln \mathcal{Z}(\beta) \tag{1.31}$$

where $\beta = 1/k_B T$ is the inverse temperature and $\mathcal{Z}$ the (Boltzmann) partition function,

$$\mathcal{Z} = \int d\Gamma e^{-\beta H} \tag{1.32}$$

where the phase space volume element is $d\Gamma = \prod_{I=1}^{N} d\phi_I d\pi_I$.

(convention: from now on, $k_B \equiv 1$)

The **specific heat** $c = \partial_T u$ is the rate of change of energy with temperature.

Easily determined here: rescale integration variables, $\phi_I \to \beta^{-1/2} X_I$, $\pi_I \to \beta^{-1/2} Y_I$, giving $\beta H(\phi, \pi) \to H(X, Y)$ indep of T (since H is quadratic). Integration measure: $d\Gamma \to \beta^{-N} d\Gamma'$, so

$$u = -\frac{1}{L} \partial_\beta \ln(\beta^{-N} K) = \rho T \tag{1.33}$$

where $\rho = N/L$ is the number density of atoms, and we have used that $K \equiv \int d\Gamma' e^{-H(X,Y)}$ is independent of T.

→temperature-independent specific heat, $c = \rho$. Note that it is **independent** of the material constants m, k_s (understandable from equipartition: N degrees of freedom, so extensive energy scales as $U = N k_B T$). Strikingly, this temperature dependence of the specific heat is not what is observed in many materials... As we will see, this points to quantum effects as dictating the low-temperature physical properties.

1.2 The quantum chain

Generally, in CM, low-energy phenomena with large T dependence →quantum mechanism.

How to quantize (1.6) ? Classically: momentum $\pi(x)$ and coordinate $\phi(x)$ are conjugate variables, $\{\pi(x), \phi(x')\} = \delta(x - x')$ (where $\{,\}$ is the Poisson bracket, and δ fn arises as the continuum generalization of discrete PB $\{P_I, R_{I'}\} = \delta_{II'}$).

Quantization: promote $\phi(x)$ and $\pi(x)$ to operators, $\phi \mapsto \hat{\phi}, \pi \mapsto \hat{\pi}$ and generalize CCR $[R_I, P_{I'}] = i\hbar\delta_{II'}$ to

$$[\hat{\phi}(x), \hat{\pi}(x')] = i\hbar\delta(x - x') \tag{1.34}$$

Operator-valued function $\hat{\phi}$ and $\hat{\pi}$ are referred to as **quantum fields**

Classical Hamiltonian density becomes quantum operator:

$$\hat{\mathcal{H}}(\hat{\phi}, \hat{\pi}) = \frac{1}{2m}\hat{\pi}^2 + \frac{k_s a^2}{2}(\partial_x \hat{\phi})^2 \tag{1.35}$$

This is not a **solution** yet, only a **formulation** in terms of field theory. We first *solve*, then *discuss* how we did it.

Fourier transform of fields:

$$\begin{pmatrix} \hat{\phi}_k \\ \hat{\pi}_k \end{pmatrix} \equiv \frac{1}{\sqrt{L}} \int_0^L dx e^{\mp ikx} \begin{pmatrix} \hat{\phi}(x) \\ \hat{\pi}(x) \end{pmatrix}, \quad \begin{pmatrix} \hat{\phi}(x) \\ \hat{\pi}(x) \end{pmatrix} \equiv \frac{1}{\sqrt{L}} \sum_k e^{\pm ikx} \begin{pmatrix} \hat{\phi}_k \\ \hat{\pi}_k \end{pmatrix}, \tag{1.36}$$

where $\sum_k$ sums over all quantized momenta $k = 2\pi m/L$, $m \in \mathbb{Z}$.

NB: the *real* classical field $\phi(x)$ quantizes to a *Hermitian* quantum field $\hat{\phi}(x)$, implying $\hat{\phi}_k = \hat{\phi}^\dagger_{-k}$ (same for $\hat{\pi}_k$). CCR become

$$[\hat{\phi}_k, \hat{\pi}_{k'}] = i\hbar\delta_{kk'} \tag{1.37}$$ CMFT(1.28)

Derivation of the Hamiltonian:

$$\int_0^L dx(\partial\hat{\phi})^2 = \sum_{k,k'}(ik\hat{\phi}_k)(ik'\hat{\phi}_{k'})\frac{1}{L}\int_0^L dx e^{i(k+k')x} = \sum_k k^2\hat{\phi}_k\hat{\phi}_{-k} = \sum_k k^2|\hat{\phi}_k|^2 \tag{1.38}$$

where we have used $\frac{1}{L}\int_0^L dx e^{-i(k+k')x} = \delta_{k+k',0}$. The Hamiltonian becomes

$$\hat{H} = \sum_k \left[\frac{1}{2m}\hat{\pi}_k\hat{\pi}_{-k} + \frac{m\omega_k^2}{2}\hat{\phi}_k\hat{\phi}_{-k}\right] \tag{1.39}$$ CMFT(1.29)

with $\omega_k = v|k|$ and $v = a\sqrt{k_s/m}$ is the classical sound wave velocity.

→Hamiltonian is a superposition of independent **harmonic oscillators** (see PRE:Phys A.2 for a revision) for the *collective* vibration modes.

1.2.1 Quasi-particle interpretation of the quantum chain

Ladder operators:

$$\hat{a}_k \equiv \sqrt{\frac{m\omega_k}{2}}(\hat{\phi}_k + \frac{i}{m\omega_k}\hat{\pi}_{-k}), \qquad \hat{a}^\dagger_k \equiv \sqrt{\frac{m\omega_k}{2}}(\hat{\phi}_{-k} - \frac{i}{m\omega_k}\hat{\pi}_k) \tag{1.40}$$ CMFT(1.32)

with generalized CCR

$$[\hat{a}_k, \hat{a}^\dagger_{k'}] = \delta_{kk'}, \qquad [\hat{a}_k, \hat{a}_{k'}] = [\hat{a}^\dagger_k, \hat{a}^\dagger_{k'}] = 0. \tag{1.41}$$ CMFT(1.33)

The Hamiltonian becomes

$$\hat{H} = \sum_k \omega_k(\hat{a}^\dagger_k\hat{a}_k + 1/2). \tag{1.42}$$ CMFT(1.34)

Here, $\omega_k \to 0$ as $k \to 0$. Excitations with this property are said to be **massless**.

Excited state of system: indexed by set $\{n_k\} = (n_1, n_2, ...)$ of quasi-particles with energy ω_k. Identified with **phonon modes** of solid.

Exercise: do CMFT 1.8.3, and get the low-temperature specific heat for a solid.

CMFT problem 1.8.3: Phonon specific heat

For the one-dimensional chain: eigenstates of system:

$$|\prod_m n_m\rangle, \qquad n_m = \#\text{phonons with } k = k_m = 2\pi m/L. \tag{1.43}$$

Total energy:

$$E_{\{n_m\}} = \sum_m \omega_{k_m}(n_m + 1/2), \qquad \omega_k = v|k|. \tag{1.44}$$

Partition function:

$$\mathcal{Z} = \mathrm{Tr} e^{-\beta \hat{H}} = \sum_{\{n_m\}} e^{-\beta E_{\{n_m\}}} = \prod_m \sum_{n_m=0}^{\infty} e^{-\beta\omega_m(n_m+1/2)} = \prod_m \frac{e^{-\beta\omega_m/2}}{1-e^{-\beta\omega_m}}. \tag{1.45}$$

so

$$\ln \mathcal{Z} = -\sum_m \left[\beta\frac{\omega_{k_m}}{2} + \ln(1-e^{-\beta\omega_{k_m}})\right]. \tag{1.46}$$

The mean energy density is thus

$$u = -\frac{1}{L}\partial_\beta \ln \mathcal{Z} = \frac{1}{L}\sum_k \left[\frac{\omega_k}{2} + \omega_k n_b(\omega_k)\right] \tag{1.47}$$

where $n_b(\omega) = \frac{1}{e^{\beta\omega}-1}$ is the Bose-Einstein distribution function. Writing this as an integral using $\sum_m \to \frac{L}{2\pi}\int dk$,

$$u = \frac{1}{2\pi}\int dk \frac{v|k|}{2} + \frac{1}{2\pi}\int dk \frac{v|k|}{e^{\beta v|k|}-1} = C_1 + \beta^{-2}C_2 \tag{1.48}$$

by scaling $k \to k/\beta$. $C_{1,2}$ are temperature-independent. We thus find

$$c_v = \partial_T u \propto T \tag{1.49}$$

If T is much larger than the highest frequency phonon mode available, we can recover the classical result $c_v = \text{cst}$ by expanding $e^{\beta v|k|} - 1 \sim \beta v|k|$.

For a d-dimensional solid: if the atoms can also move in d dimensions, then the displacements and conjugate momenta become vectors. The interaction term is

$$\frac{k_s}{2}\sum_{i=1}^{d}\left(\boldsymbol{\phi}_{\mathbf{I}+\mathbf{e}_i} - \boldsymbol{\phi}_{\mathbf{I}}\right)^2 \tag{1.50}$$

where $\mathbf{e}_i$ are unit vectors. In discrete variables, the Hamiltonian is

$$H = \sum_{\mathbf{I}}\left[\frac{\boldsymbol{\pi}_{\mathbf{I}}^2}{2m} + \frac{k_s}{2}\sum_{i=1}^{d}\left(\boldsymbol{\phi}_{\mathbf{I}+\mathbf{e}_i} - \boldsymbol{\phi}_{\mathbf{I}}\right)^2\right] \tag{1.51}$$

and in the continuum limit,

$$\hat{H} = \int d^d x \sum_{i=1}^{d}\left[\frac{\pi_i(\mathbf{x})^2}{2m} + \frac{k_s a^2}{2}(\nabla_i\hat{\boldsymbol{\phi}})^2\right] \tag{1.52}$$

Fourier transform: operator commutation relations become

$$[\hat{\phi}_{i,\mathbf{k}}, \hat{\pi}_{j,\mathbf{k}'}] = i\hbar\delta_{i,j}\delta_{\mathbf{k},\mathbf{k}'} \tag{1.53}$$

Ladder operators:

$$\boldsymbol{a}_{\mathbf{k}} = \sqrt{\frac{m\omega_{\mathbf{k}}}{2}}\left(\hat{\boldsymbol{\phi}}_{\mathbf{k}} + \frac{i}{m\omega_{\mathbf{k}}}\hat{\boldsymbol{\pi}}_{-\mathbf{k}}\right) \tag{1.54}$$

Hamiltonian in terms of ladder operators:

$$\hat{H} = \sum_{\mathbf{k}}\sum_{i=1}^{d}\omega_{\mathbf{k}}(a^{\dagger}_{i,\mathbf{k}}a_{i,\mathbf{k}} + 1/2) \tag{1.55}$$

where $\omega_{\mathbf{k}} = a\sqrt{\frac{k_s}{m}}|\mathbf{k}| \equiv v|\mathbf{k}|$ and the momenta are quantized according to $\mathbf{k} = \frac{2\pi}{L}\mathbf{m}$ with $\mathbf{m} = (m_1, ..., m_d)$. Eigenstates and their energies are given by

$$|\prod_i\prod_{\mathbf{m}} n_{i,\mathbf{m}}\rangle, \qquad E_{\{n_{i,\mathbf{m}}\}} = \sum_i\sum_{\mathbf{m}}\omega_{\mathbf{k}_\mathbf{m}}(n_{i,\mathbf{m}} + 1/2) \tag{1.56}$$

Partition function:

$$\mathcal{Z} = \ \mathrm{Tr}\ e^{-\beta\hat{H}} = \prod_i\prod_{\mathbf{m}} e^{-\beta\omega_{\mathbf{k}_\mathbf{m}}(n_{i,\mathbf{m}}+1/2)} \tag{1.57}$$

so

$$\ln\mathcal{Z} = -\sum_i\sum_{\mathbf{m}}\left[\beta\frac{\omega_{\mathbf{k}_\mathbf{m}}}{2} + \ln(1 - e^{-\beta\omega_{\mathbf{k}_\mathbf{m}}})\right] \to -\left(\frac{L}{2\pi}\right)^d d\int d^dk\left[\beta\frac{\omega_{\mathbf{k}}}{2} + \ln(1 - e^{-\beta\omega_{\mathbf{k}}})\right] \tag{1.58}$$

and therefore the free energy per unit site is

$$u = -\frac{1}{L^d}\partial_\beta\ln\mathcal{Z} = d\int\frac{d^dk}{(2\pi)^d}\left[\frac{\omega_{\mathbf{k}}}{2} + \frac{\omega_{\mathbf{k}}}{e^{\beta\omega_{\mathbf{k}}} - 1}\right] \equiv u_0 + u_1, \tag{1.59}$$

with u_0 T independent, and

$$u_1 = \int\frac{d^dk}{(2\pi)^d}\frac{v_F d|\mathbf{k}|}{e^{\beta\omega_{\mathbf{k}}} - 1} = \beta^{-d-1}\int\frac{d^dk}{(2\pi)^d}\frac{v_F d|\mathbf{k}|}{e^{\omega_{\mathbf{k}}} - 1} = \beta^{-d-1}\bar{u}_1 \tag{1.60}$$

with $\bar{u}_1$ T independent. Therefore, the specific heat goes like

$$c_V = \partial_T u \propto T^d. \tag{1.61}$$

CMFT problem 1.8.4: Van der Waals force

$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + \frac{m\omega_0^2}{2}(\hat{x}_1^2 + \hat{x}_2^2) + mK\hat{x}_1\hat{x}_2 \tag{1.62}$$

where the last term represents the dipole-dipole interaction, and $K(r) = \frac{qe^2}{mr^3}$ encapsulates the details of the interaction.

Spectrum: interaction can be written

$$\hat{U} = \hat{x}^T A \hat{x}, \qquad \hat{x} \equiv \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \qquad A \equiv \frac{m}{2}\begin{pmatrix} \omega_0^2 & K \\ K & \omega_0^2 \end{pmatrix}. \tag{1.63}$$

New eigenvalues: $\omega_\pm = (\omega_0^2 \pm K)^{1/2}$. Ground state:

$$E_0 = \frac{\omega_-}{2} + \frac{\omega_+}{2} = \frac{1}{2}(\sqrt{\omega_0^2 - K} + \sqrt{\omega_0^2 + K}) = \omega_0 - \frac{K^2}{8\omega_0^3} + ... \tag{1.64}$$

so the reduction in energy is by a factor $V = \frac{K^2}{8\omega_0^3}$.

Classical polarizability: $V = \frac{q^2e^4\omega_0 m^2\alpha^2}{m^2r^6 8e^4} = \frac{q^2\omega_0\alpha^2}{8r^6}$ where $\alpha = \frac{e^2}{m\omega_0^2}$. But $\langle q^2\rangle = 2$, and with a factor of 3 since we're in three dimensions, we get

$$V = -\frac{3\omega_0\alpha^2}{4r^6}. \tag{1.65}$$

Supplement: Maxwell's equations as a variational principle

For classical electrodynamics: inhomogeneous Maxwell equations:

$$\nabla \cdot \mathbf{E} = \rho, \qquad \nabla \times \mathbf{B} - \partial_t \mathbf{E} = \mathbf{j} \tag{1.66}$$

(simplicity: vacuum theory, so $\mathbf{E} = \mathbf{D}$ and $\mathbf{B} = \mathbf{H}$). We've set $c = 1$. These can be obtained from a variational principle, in which the homogeneous equations:

$$\nabla \times \mathbf{E} + \partial_t \mathbf{B} = 0, \qquad \nabla \cdot \mathbf{B} = 0 \tag{1.67}$$

are regarded as *ab initio* constraints on the 'degrees of freedom' $\mathbf{E}, \mathbf{B}$.

Need (1) a field formulated in terms of suitable 'coordinates', and (2) its action.

Natural 'coordinates': EM 4-potential $A_\mu = (\phi, -\mathbf{A})$. A is unconstrained and gives fields $\mathbf{E}, \mathbf{B}$ through $\mathbf{E} = -\nabla\phi - \partial_t \mathbf{A}$, $\mathbf{B} = \nabla \times \mathbf{A}$. These are 'overly free' since gauge transformations $A_\mu \to A_\mu + \partial_\mu \Gamma$ leave fields invariant.

Better notation: use

$$F = \{F_{\mu\nu}\} = \begin{bmatrix} 0 & E_1 & E_2 & E_3 \\ -E_1 & 0 & -B_3 & B_2 \\ -E_2 & B_3 & 0 & -B_1 \\ -E_3 & -B_2 & B_1 & 0 \end{bmatrix} \tag{1.68}$$

so now $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ where $x_\mu = (t, -\mathbf{x})$ and $\partial_\mu = (\partial_t, \nabla)$.

Finding the action: could postulate an action that reproduces Maxwell's equation. More elegant strategy: find a symmetry that defines structure of the action. Here: *Lorentz invariance.*

Lorentz invariance: a linear transformation $T_{\mu\nu}$ is a Lorentz transformation $X_\mu \to X'_\mu \equiv T_{\mu\nu} X_\nu$ if it leaves the 4-metric $g = diag(1, -1, -1, -1)$ invariant. Notation: $X^\mu = g^{\mu\nu} X_\nu$, so Lorentz invariance: $X^\mu X_\mu = X'^\mu X'_\mu$.

Use symmetry criterion to conjecture form of action from 3 assumptions (all indep of Maxwell): action should be invariant under (a) Lorentz and (b) gauge transformations, and (c) it should be simple (local, ...). Most elementary choice:

$$S[A] = \int d^4x (c_1 F_{\mu\nu} F^{\mu\nu} + c_2 A_\mu j^\mu) \tag{1.69}$$

CMFT(1.22)

with $d^4x = \prod_\mu dx_\mu$, $j_\mu = (\rho, -\mathbf{j})$ and $c_{1,2}$ are constants to be determined. This is the only structure compatible with the requirements, to quadratic order in A.

Variational principle:

$$\frac{\partial \mathcal{L}}{\partial A_\mu} - \partial_\nu \frac{\partial \mathcal{L}}{\partial(\partial_\nu A_\mu)} = 0, \qquad \mu = 0, ..., 3. \tag{1.70}$$

CMFT(1.23)

with $S = \int d^4x \mathcal{L}$. In equations of motion: $\partial_{A_\mu} \mathcal{L} = c_2 j^\mu$, $\partial_{\partial_\nu A_\mu} \mathcal{L} = -4c_1 F^{\mu\nu}$. This gives $4c_1 \partial^\nu F_{\nu\mu} = c_2 j_\mu$. We thus get Maxwell for $c_1/c_2 = 1/4$, and the correct energy density for $c_1 = -1/4$, so

$$\mathcal{L}(A_\mu, \partial_\nu A_\mu) = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + A_\mu j^\mu \tag{1.71}$$

CMFT(1.24)

is the **Lagrangian of the electromagnetic field**.

Remarkable achievement: by invoking only symmetry, we've found the structure of Maxwell's equation. Relativistic invariance is in-built. We've also shown that these are the *only* equations of motion linear in current-density which are consistent with this invariance.

Summary: two approaches for getting a field theory:

• **Microscopic analysis**: starting from a microscopic theory, project onto important degrees of freedom for low-energy dynamics.
Advantages: rigorous, fixes all constants.
Disadvantages: time-consuming, often not viable for complex systems.

• **Symmetry method**: infer effective theory on basis of fundamental symmetries only.
Advantages: fast, elegant.
Disadvantages: less explicit than microscopic approach, does not fix coefficients.

Supplement: Noether's theorem in field theory

Basic paradigm: **continuous symmetry →conservation law**.

Ex.: rotational symetry ↔conservation of angular momentum

Tool to identify conservation laws from symmetries: Noether's theorem.

Symmetry transformation: two pieces of data.
First, a mapping $M \to M, x \mapsto x'(x)$ (automorphism of base manifold).
Second: transformation of field configurations, $(\phi : M \to T) \mapsto (\phi' : M \to T)$ defining transformed values $\phi'(x') = F[\{\phi(x)\}]$ in terms of the "old" field ϕ.

Example: translations in space-time. $x' = x + a$, $a \in \mathbb{R}^m$, $\phi'(x') = \phi(x)$. Translation invariant system iff $S[\phi] = S[\phi']$.

Other example: rotational symmetry: $x' = Rx$ with $R \in O(m)$ a rotation in Euclidean space-time. Here, $\phi'(x') = \phi(x)$ would be unphysical. Properly rotated field configuration: $\phi'(x') = R\phi(x)$.

My own derivation... Any finite symmetry transformation can be obtained from a series of infinitesimal transformations, which we consider. We have already seen what the variation of the action is under a change of the field. Using the notation

$$\phi^i(x) \to \phi'^i(x) = \phi^i(x) + \delta\phi^i(x), \tag{1.72}$$

we had (provided the field obeyed the Euler-Lagrange equation)

$$\delta_\phi S = \int_{\partial M} d^{m-1}\sigma_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^i} \delta\phi^i \tag{1.73}$$

Consider now changing the *coordinates* according to

$$x_\mu \to x'_\mu = x_\mu + \delta x_\mu \tag{1.74}$$

The change in the action coming from such a coordinate change occurs at the boundary, *i.e.*

$$\begin{aligned} \delta_x S &= \int d^m x' \mathcal{L}' - \int d^m x \mathcal{L} = \int d^m x [(1 + \partial_\mu \delta x^\mu)(\mathcal{L} + \partial_\mu \mathcal{L} \delta x^\mu) - \mathcal{L}] \\ &= \int d^m x \partial_\mu (\mathcal{L} \delta x^\mu) + \mathcal{O}(\delta^2) = \int_{\partial M} d^{m-1}\sigma_\mu \mathcal{L} \delta x^\mu + \mathcal{O}(\delta^2) \end{aligned} \tag{1.75}$$

The total variation of the action under both coordinate and field change is thus

$$\delta S = \int_{\partial M} d^{m-1}\sigma_\mu \left[\frac{\partial \mathcal{L}}{\partial \partial_\mu \phi^i} \delta\phi^i + \mathcal{L} \delta x^\mu \right]. \tag{1.76}$$ deltaS

Derivation in CMFT notation

In the notation of CMFT, the transformation is written as

$$x_\mu \to x'_\mu = x_\mu + \frac{\partial x_\mu}{\partial \omega_a}|_{\omega=0}\omega_a(x),$$
$$\phi^i(x) \to \phi^{'i}(x') = \phi^i(x) + \omega_a(x)F^i_a[\phi] \tag{1.77}$$

where $\{\omega_a\}$ is a set of parameter functions characterizing the transformation. We now calculate the change in the action (CMFT(1.16) CMFT(1.42) 1.22) under (1.77):

$$\Delta S = \int d^m x' \mathcal{L}(\phi^{'i}(x'), \partial_{x'_\mu}\phi^{'i}(x')) - \int d^m x \mathcal{L}(\phi^i(x), \partial_{x_\mu}\phi^i(x)) \tag{1.78}$$

From (CMFT(1.42) 1.77),

$$\frac{\partial x'_\mu}{\partial x^\nu} = \delta_{\mu\nu} + \frac{\partial}{\partial x^\nu}(\omega_a \frac{\partial x_\mu}{\partial \omega_a}) \tag{1.79}$$

and using

$$|\frac{\partial x'_\mu}{\partial x_\nu}| = 1 + \frac{\partial}{\partial x_\mu}(\omega_a \frac{\partial x_\mu}{\partial \omega_a}) + O(\omega^2) \tag{1.80}$$

we get $\partial_\mu = \frac{\partial}{\partial x^\mu}$)

$$\Delta S \backsimeq \int d^m x \left[(1 + \partial_\mu(\omega_a \partial_{\omega_a} x^\mu)\mathcal{L}(\phi^i + F^i_a\omega_a, (\delta^\nu_\mu - \partial_\mu(\omega_a\partial_{\omega_a}x^\nu))\partial_\nu(\phi^i + F^i_a\omega_a)) \right.$$
$$\left. -\mathcal{L}(\phi^i(x), \partial_\mu\phi^i(x))\right] \tag{1.81}$$

Going further, we have

$$\Delta S \backsimeq \int d^m x \left[(\partial_\mu(\omega_a\frac{\partial x^\mu}{\partial\omega_a}))\mathcal{L} + \frac{\partial\mathcal{L}}{\partial\phi^i}F^i_a\omega_a + \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)}\left[\partial_\mu(F^i_a\omega_a) - (\partial_\mu(\omega_a\frac{\partial x^\nu}{\partial\omega_a}))\partial_\nu\phi^i\right]\right]$$
$$= \int d^m x \left[(\frac{\partial\mathcal{L}}{\partial\phi^i} - \partial_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)})F^i_a\omega_a + (\partial_\mu(\omega_a\frac{\partial x^\mu}{\partial\omega_a}))\mathcal{L} + \omega_a\frac{\partial x^\nu}{\partial\omega_a}\partial_\mu(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)}\partial_\nu\phi^i) + \right.$$
$$\left. +\partial_\mu\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)}F^i_a\omega_a - \omega_a\frac{\partial x^\nu}{\partial\omega_a}\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)}\partial_\nu\phi^i\right]\right] \tag{1.82}$$

But we have

$$\partial_\nu\mathcal{L} = \frac{\partial\mathcal{L}}{\partial\phi^i}\partial_\nu\phi^i + \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)}\partial_\mu\partial_\nu\phi^i = (\partial_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)})\partial_\nu\phi^i + \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)}\partial_\mu\partial_\nu\phi^i$$
$$= \partial_\mu\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)}\partial_\nu\phi^i\right] \tag{1.83}$$

where we have made use of the Euler-Lagrange equation for the field. We thus find

$$\Delta S = \int d^m x \partial_\mu\left[\omega_a\left(\mathcal{L}\frac{\partial x^\mu}{\partial\omega_a} - \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)}\partial_\nu\phi^i\frac{\partial x^\nu}{\partial\omega_a} + \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi^i)}F^i_a\right)\right] \equiv -\int d^m x j^a_\mu(x)\partial_\mu\omega_a. \tag{1.84}$$

To check the correspondent of this to equation (deltaS 1.76), note that the notation correspondence between the 'easy' and CMFT field and coordinate parametrization is

$$\delta x_\mu = \frac{\partial x_\mu}{\partial\omega_a}|_{\omega=0}\omega_a(x),$$
$$\delta\phi^i(x) = \phi^{'i}(x) - \phi^i(x) = \phi^{'i}(x') - \phi^i(x) + \phi^{'i}(x) - \phi^{'i}(x')$$
$$= \omega_a(x)F^i_a - \frac{\partial x_\mu}{\partial\omega_a}|_{\omega=0}\omega_a(x)\frac{\partial\phi^i}{\partial x_\mu} + O(\omega^2) \tag{1.85}$$

Putting this back into δS (1.76) above yields back (1.84).

Back to CMFT notation This means that we can rewrite the variation of the action as

$$\Delta S = -\int_{\partial M} d^{m-1}\sigma^{\mu}\omega_a(x) j^a_{\mu}(x) \tag{1.86}$$

where

$$j^a_{\mu} = \left(\frac{\partial \mathcal{L}}{\partial(\partial^{\mu}\phi^i)}\partial_{\nu}\phi^i - \mathcal{L}\delta_{\mu\nu}\right)\frac{\partial x^{\nu}}{\partial \omega_a}|_{\omega=0} - \frac{\partial \mathcal{L}}{\partial(\partial^{\mu}\phi^i)}F^i_a \tag{1.87}$$

CMFT(1.43)

where the term in first parentheses is known as the **energy-momentum tensor** $T_{\mu\nu}$.

If the action is invariant under an arbitrary set of functions ω_a, we have that

$$\int_{\partial M} d^{m-1}\sigma^{\mu} j^a_{\mu} = 0 \tag{1.88}$$

or, by using the multidimensional version of Gauss's theorem,

$$\int_{M} d^m x \partial^{\mu} j^a_{\mu} = 0 \tag{1.89}$$

Since we really can choose M as we wish, we therefore obtain a conserved current j^a_{μ} !

Thus: **Noether's theorem: a continuous symmetry entails a classically conserved current.**

In Euclidean $(1+d)$-dimensional space-time, we can therefore define a conserved charge

$$Q^a \equiv \int d^d x j^a_0,$$

$$\partial_t Q^a \equiv \partial_0 Q^a = \int d^d x \partial_0 j^a_0 = -\int d^d x \partial_i j^a_i = \int_{\partial D} j^a = 0; \tag{1.90}$$

where we have used Gauss's theorem again and assumed that the current density vanishes at spatial infinity.

Example: translational invariance Take

$$x'_{\mu} = x_{\mu} + a_{\mu}, \qquad \phi'(x') = \phi(x). \tag{1.91}$$

The Noether current is then

$$T^{\mu}_{\nu}(x) = \frac{\partial \mathcal{L}}{\partial(\partial_{\mu}\phi^i)}\partial_{\nu}\phi^i - \mathcal{L}\delta^{\mu}\nu. \tag{1.92}$$

with conserved charges

$$P_{\nu} \equiv \int d^d x \left(\frac{\partial \mathcal{L}}{\partial(\partial_0\phi^i)}\partial_{\nu}\phi^i - \mathcal{L}\delta_{0\nu}\right). \tag{1.93}$$

Chapter 2

The operator formalism

OF

Experience shows that the solution to a physical problem often becomes transparent when one uses the correct language to formulate it. This chapter introduces an operator-based formalism for many-body quantum systems often referred to as 'second quantization'[1]. The idea is that instead of working with many-body wavefunctions, we work directly with operators that 'create' them on a specified reference state (the 'vacuum').

2.1 Many-body wavefunctions

Let's imagine that we have some quantum problem associated to a certain Hamiltonian $\hat{H}$ (for example, a particle in a box). By solving the Schrödinger equation for a single particle, one gets a set of normalized wavefunctions $\{|\psi_i\rangle\}$ (with real-space representation $\psi_i(x) = \langle x|\psi_i\rangle$), such that $\hat{H}|\psi_i\rangle = \varepsilon_i|\psi_i\rangle$. For purposes of discussion, we'll assume that the one-body Hilbert space has a basis of states $|i\rangle$ which are indexed by an integer $i = 1, 2, ...$ (not necessarily eigenstates; they are just assumed to form a basis).

If we now consider putting two identical particles in such a system, according to the postulates of quantum mechanics (more precisely: Pauli's principle), we must symmetrize or antisymmetrize the wavefunction depending on whether the particles are bosons or fermions. The normalized real-space two-particle wavefunctions of fermions or bosons in states i_1, i_2 are then respectively given by (up to an arbitrary overall phase)

$$\begin{aligned}\Psi_F(x_1, x_2|i_1, i_2) &= \frac{1}{\sqrt{2}}\left(\langle x_1|i_1\rangle\langle x_2|i_2\rangle - \langle x_1|i_2\rangle\langle x_2|i_1\rangle\right), \\ \Psi_B(x_1, x_2|i_1, i_2) &= \frac{1}{\sqrt{2}}\left(\langle x_1|i_1\rangle\langle x_2|i_2\rangle + \langle x_1|i_2\rangle\langle x_2|i_1\rangle\right). \end{aligned} \tag{2.1}$$

Omitting the spatial coordinates by working directly in Dirac bracket notation gives the simpler form

$$|i_1, i_2\rangle_{F(B)} \equiv \frac{1}{\sqrt{2}}\left(|i_1\rangle \otimes |i_2\rangle + \zeta|i_2\rangle \otimes |i_1\rangle\right) \tag{2.2}$$

with $\zeta = -1$ for fermions and $\zeta = 1$ for bosons. Note that the wavefunctions obey the correct symmetries under exchange of particle coordinates:

$$\Psi_B(x_2, x_1|i_1, i_2) = \Psi_B(x_1, x_2|i_1, i_2), \qquad \Psi_F(x_2, x_1|i_1, i_2) = -\Psi_F(x_1, x_2|i_1, i_2), \tag{2.3}$$

[1] Frankly, a stupid name for a good idea. There is no 'second' quantization, just the usual one. Here, we'll use the more descriptive term 'operatorial quantization'.

but that in these conventions, this is also true upon exchange of the state indices:

$$\Psi_B(x_1,x_2|i_2,i_1)=\Psi_B(x_1,x_2|i_1,i_2),\qquad \Psi_F(x_1,x_2|i_2,i_1)=-\Psi_F(x_1,x_2|i_1,i_2). \tag{2.4}$$

In the general N-body case, assuming that states $i_1,...,i_N$ are occupied, the wavefunction is written as

$$|i_1,i_2,...,i_N\rangle \equiv \frac{1}{[N!\prod_{j=0}^{\infty} n_j!]^{1/2}}\sum_{\mathcal{P}} \zeta^{(1-\mathrm{sgn}\mathcal{P})/2}|i_{\mathcal{P}_1}\rangle\otimes|i_{\mathcal{P}_2}\rangle\otimes...\otimes|i_{\mathcal{P}_N}\rangle \tag{2.5}$$ CMFT(2.1)

with n_j the number of particles in state j (for fermions, this is restricted to 0 or 1). The summation runs over the $N!$ permutations of the set of 'occupied' quantum numbers $\{i_1,...,i_N\}$ (note that in the bosonic case, there can be multiple entries of the same level), and sgn$\mathcal{P}$ is the sign of the permutation.

For the specific case of fermions, this permutation sum has the structure of a determinant, which is known as the **Slater determinant**.

To fix conventions completely, we have to rely on the explicit ordering of the numbers $i_1,...,i_N$ and for example agree that the first term in the sum (with coefficient $+1$) is the one corresponding to the indices i_a begin given in increasing order. There is however no 'physics' in this convention (it's just a convention!).
At first sight, one expects N-body quantum mechanics to take place in the simple tensor product space

$$\mathcal{H}^N \equiv \underbrace{\mathcal{H}\otimes\mathcal{H}\otimes...\otimes\mathcal{H}}_{N\text{ times}}. \tag{2.6}$$

The symmetrization postulate of quantum mechanics however requires our wavefunctions to form a representation of the permutation group S^N: $\mathcal{H}^N\to\mathcal{H}^N$, $|i_1\rangle\otimes...\otimes|i_N\rangle\to|i_{P_1}\rangle\otimes...\otimes|i_{P_N}\rangle$. S^N has two simple one-dimensional irreducible representations: the symmetric $P(\psi)=\psi$, and the antisymmetric $P(\psi)=$ sgn $(\psi)\psi$. Quantum mechanics postulates that bosons/fermions transform respectively according to the identity/alternating representations[2]. Our states thus really belong to a subset $\mathcal{F}^N\subset\mathcal{H}^N$ having the right symmetry: this is known as the **physical Hilbert space**. Obtaining a basis of $\mathcal{F}^N$ is straightforwardly done by applying symmetrization/antisymmetrization operators, $P^s=\sum_P P$ or $P^a=\sum_P$ sgn $(P)P$, to a basis of $\mathcal{H}^N$.

There are many practical reasons why the form (CMFT(2.1) 2.5) of our many-body wavefunction is not convenient:

• Computing the overlap of two wavefunctions requires handling $(N!)^2$ different products.

• This representation is for fixed particle number N. In applications however, we want to let N change (thinking of averaging over a grand-canonical ensemble for example, or of physical processes where particles are added/removed from a system).

Thinking about the content of equation (CMFT(2.1) 2.5), as evident form the left-hand side, the *information* required to specify it is simply the set $\{i_1,...,i_N\}$. This set however can be rewritten in terms of the occupation numbers of each available state. If we denote by n_i the number of

[2]In two dimensions, other possibilities exist, since one must then look at representations of the braid group. Particles with other statistics (neither bosonic nor fermionic) then exist, which are known as anyons.

'times' state i appears, we have the equivalence

$$\{i_1, ..., i_N\} \leftrightarrow \{n_1, n_2, ...\} \text{ with } \sum_j n_j = N. \tag{2.7}$$

This leads us to consider general states in the **occupation number representation**,

$$|n_1, n_2, ...\rangle, \qquad n_j = 0, 1 \text{ (fermions) or } \; n_j = 0, 1, 2, ... \text{ (bosons)} \tag{2.8}$$

without constraint on $\sum_j n_j$. These states form a basis of the **Fock space**

$$\mathcal{F} \equiv \oplus_{N=0}^{\infty} \mathcal{F}^N \tag{2.9}$$ CMFT(2.2)

in the sense that any wavefunction of any (conbination of different) numbers of particles can be written as the linear combination

$$|\Psi\rangle = \sum_{n_1, n_2, ...} c_{n_1, n_2, ...} |n_1, n_2, ...\rangle, \qquad c_{\mathbf{n}} \in \mathbb{C}. \tag{2.10}$$

One special object in Fock space is the state associated to the physical Hilbert space with zero particles $\mathcal{F}^0$. This space is a dimension-one Hilbert space, and its basis element, known as the **vacuum state**, is traditionally denoted by $|0\rangle$. The Fock space is the principal arena of quantum many-body theory, and the vacuum state is the foundation on which it is built.

2.1.1 Creation and annihilation operators

Since a many-body wavefunction such as (2.5) is fully defined by specifying the set of occupied one-body states, we can imagine that it is built up from adding particles in the relevant states one at a time, starting from the vacuum state. To implement this idea, we thus define a set of operators acting in Fock space in the following way. For every $i = 1, 2, ...$, we define 'raising' operators $a_i^\dagger : \mathcal{F} \to \mathcal{F}$ through the relation

$$a_i^\dagger |n_1, ..., n_i, ...\rangle \equiv (n_i + 1)^{1/2} \zeta^{s_i} |n_1, ..., n_i + 1, ...\rangle \tag{2.11}$$ CMFT(2.3)

with $s_i = \sum_{j=1}^{i-1} n_j$ being a (convention-defined) statistical sign. The central idea is that starting from the vacuum state, we are able to generate every basis state of $\mathcal{F}$ by repeated applications of $a_i^\dagger$:

$$|n_1, n_2, ...\rangle = \prod_i \frac{1}{\sqrt{n_i!}} (a_i^\dagger)^{n_i} |0\rangle \tag{2.12}$$ CMFT(2.4)

(in this equation, with our convention (2.11), the product is taken left to right for increasing i; this is once again not 'physical', just conventional).

Without seeming to do much, we are actually overhauling our way of dealing with wavefunctions. The complicated permutation sum in (2.5) is generated *automatically* by the $a_i^\dagger$ operators, which are called **creation operators**. Instead of viewing our wavefunctions as a very complicated (anti)symmetrized sum of basis vectors, we view them as a product of creation operators on the vacuum.

A crucial consequence of the defining operator commutation relations (CMFT(2.3) 2.11) is that the creation operators obey the relation $(a_i^\dagger a_j^\dagger - \zeta a_j^\dagger a_i^\dagger)|n_1, n_2, ...\rangle = 0$. Since this in fact holds for all basis vectors, we can promote this to the operator identity

$$[a_i^\dagger, a_j^\dagger]_\zeta = 0, \qquad \text{where } [\hat{A}, \hat{B}]_\zeta \equiv \hat{A}\hat{B} - \zeta \hat{B}\hat{A}. \tag{2.13}$$

Our creation operators thus obey (anti)commutation relations reflecting the statistics of the quantum particles they represent.

To complete the set of operators, we need the adjoints of our creation operators. From complex conjugate of (CMFT(2.3) 2.11), we get the matrix elements of the $a^\dagger$ operator:

$$\langle n_1, ..., n_i, ...|a_i^\dagger|n_1', ..., n_i', ...\rangle = (n_i' + 1)^{1/2} \zeta^{s_i'} \delta_{n_1 n_1'} ... \delta_{n_i, n_i'+1} \tag{2.14}$$

so

$$\langle n_1', ..., n_i', ...|a_i|n_1, ..., n_i, ...\rangle^* = n_i^{1/2} \zeta^{s_i} \delta_{n_1' n_1} ... \delta_{n_i', n_i - 1} ... \tag{2.15}$$

Since this holds for any bra, we thus have

$$a_i|n_1, ..., n_i, ...\rangle = n_i^{1/2} \zeta^{s_i} |n_1, ..., n_i - 1, ...\rangle \tag{2.16}$$ CMFT(2.6)

so the a_i are **annihilation operators**. Note in particular that the vacuum is annihilated by any of the annihilation operators,

$$a_i|0\rangle = 0. \tag{2.17}$$

Summarizing, the creation operators 'hop' us in Fock space from each fixed-N physical Hilbert space to the $N+1$ one, $a^\dagger : \mathcal{F}^N \to \mathcal{F}^{N+1}$, whereas the annihilation operators bring us back down, $a : \mathcal{F}^N \to \mathcal{F}^{N-1}$.

A simple calculation shows that the creation and annihilation operators obey the following mutual relations:

$$[a_i, a_j^\dagger]_\zeta = \delta_{ij}, \qquad [a_i, a_j]_\zeta = 0, \qquad [a_i^\dagger, a_j^\dagger]_\zeta = 0. \tag{2.18}$$ CMFT(2.7)

To summarize: instead of working with (CMFT(2.1) 2.5) and its factorially large number of terms, we shall work with states constructed by 'raising' the vacuum with our creation operators, (CMFT(2.4) 2.12). All (anti)symmetrization requirements are then automatically taken care of by the canonical (anti)commutation relations (CMFT(2.7) 2.18).

Practicalities From now on: only use Greek letters λ as label for single-particle states instead of integers.

• **Change of basis** Resolution of identity: $\mathbf{1} = \sum_{\lambda=0}^{\infty} |\lambda\rangle\langle\lambda|$. This means that $|\tilde{\lambda}\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\tilde{\lambda}\rangle$ with $|\lambda\rangle = a_\lambda^\dagger|0\rangle$ and $|\tilde{\lambda}\rangle = a_{\tilde{\lambda}}^\dagger|0\rangle$, so

$$a_{\tilde{\lambda}}^\dagger = \sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a_\lambda^\dagger, \qquad a_{\tilde{\lambda}} = \sum_\lambda \langle\tilde{\lambda}|\lambda\rangle a_\lambda. \tag{2.19}$$ CMFT(2.8)

Often: continuous sets of quantum numbers. Then, sums go into integrals. Example: Fourier representation:

$$a_k = \int_0^L dx \langle k|x\rangle a(x), \qquad a(x) = \sum_k \langle x|k\rangle a_k, \qquad \langle k|x\rangle = \langle x|k\rangle^* = e^{-ikx}/\sqrt{L}. \tag{2.20}$$ CMFT(2.9)

2.1.2 Representation of physical operators

Our set of creation/annihilation operators is sufficient to allow us to navigate through the whole Fock space. This means that an arbitrary operator in Fock space can be written as a combination of creation/annihilation operators. The structure of a generic operator is sketched as follows:

$$\hat{O} = (\text{put particles back in})(\text{operator matrix element})(\text{remove particles involved}). \quad (2.21)$$ eq:OF:Ostruct

For fermions, we have to take care of the order in which these removing/putting back in operations are performed. A few examples are best to illustrate the general idea.

The simplest case to consider is that of **one-body operators** acting in $\mathcal{F}^N$: $\hat{\mathcal{O}}_1 = \sum_{n=1}^N \hat{o}_n$, with $\hat{o}_n$ an ordinary single-particle operator acting on the n-th particle, *e.g.* kinetic energy $\hat{T} = \sum_n \frac{\hat{p}_n^2}{2m}$, or one-body potential $\hat{V} = \sum_n V(\hat{x}_n)$, or spin operator $\sum_n \hat{\mathbf{S}}_n$.

Define the **occupation number operator**

$$\hat{n}_\lambda = a_\lambda^\dagger a_\lambda \quad (2.22)$$ CMFT(2.10)

with $\hat{n}_\lambda (a_\lambda^\dagger)^n|0\rangle = n(a_\lambda^\dagger)^n|0\rangle$. Since $\hat{n}_\lambda$ commutes with all $a_{\lambda'\neq\lambda}^\dagger$, we have $\hat{n}_\lambda|n_{\lambda_1}, n_{\lambda_2}, ...\rangle = n_\lambda|n_{\lambda_1}, n_{\lambda_2}, ...\rangle$. Consider now for simplicity a one-body operator $\hat{\mathcal{O}}_1$ whose single-particle operators $\hat{o}_n$ are diagonal in the basis $|\lambda\rangle$, that is $\hat{o} = \sum_i \hat{o}|\lambda_i\rangle\langle\lambda_i| = \sum_i o_{\lambda_i}|\lambda_i\rangle\langle\lambda_i|$ with $o_{\lambda_i} = \langle\lambda_i|\hat{o}|\lambda_i\rangle$. Then,

$$\begin{aligned}\langle n'_{\lambda_1}, n'_{\lambda_2}, ...|\hat{\mathcal{O}}_1|n_{\lambda_1}, n_{\lambda_2}, ...\rangle &= \langle n'_{\lambda_1}, n'_{\lambda_2}, ...| \sum_n \hat{o}_n |n_{\lambda_1}, n_{\lambda_2}, ...\rangle \\ &= \langle n'_{\lambda_1}, n'_{\lambda_2}, ...| \sum_i o_{\lambda_i} n_{\lambda_i} |n_{\lambda_1}, n_{\lambda_2}, ...\rangle = \langle n'_{\lambda_1}, n'_{\lambda_2}, ...| \sum_i o_{\lambda_i} \hat{n}_{\lambda_i} |n_{\lambda_1}, n_{\lambda_2}, ...\rangle. \quad (2.23)\end{aligned}$$

Since this holds for any set of states, we get

$$\hat{\mathcal{O}}_1 = \sum_\lambda o_\lambda \hat{n}_\lambda = \sum_\lambda \langle\lambda|\hat{o}|\lambda\rangle \hat{n}_\lambda. \quad (2.24)$$

This can be written back in a general basis by using the transformation rule $a_\lambda^\dagger = \sum_\mu \langle\mu|\lambda\rangle a_\mu^\dagger$ and its h.c.:

$$\begin{aligned}\hat{\mathcal{O}}_1 &= \sum_\lambda \langle\lambda|\hat{o}|\lambda\rangle a_\lambda^\dagger a_\lambda = \sum_{\lambda\mu\nu} \langle\lambda|\hat{o}|\lambda\rangle\langle\mu|\lambda\rangle\langle\lambda|\nu\rangle a_\mu^\dagger a_\nu = \sum_{\lambda\mu\nu} o_\lambda \langle\lambda|\lambda\rangle\langle\mu|\lambda\rangle\langle\lambda|\nu\rangle a_\mu^\dagger a_\nu \\ &= \sum_{\lambda\mu\nu} o_\lambda \langle\mu|\lambda\rangle\langle\lambda|\nu\rangle a_\mu^\dagger a_\nu = \sum_{\mu\nu} \langle\mu|\hat{o}\left(\sum_\lambda |\lambda\rangle\langle\lambda|\right)|\nu\rangle a_\mu^\dagger a_\nu = \sum_{\mu\nu} \langle\mu|\hat{o}|\nu\rangle a_\mu^\dagger a_\nu. \quad (2.25)\end{aligned}$$

Examples 1) Spin operator $S^i_{\alpha\alpha'} = \frac{\sigma^i_{\alpha\alpha'}}{2}$ with α, α' two-component spin indices and σ the Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.26)$$ CMFT(2.12)

The **spin operator** assumes the form

$$\hat{\mathbf{S}} = \sum_\lambda a_{\lambda\alpha'}^\dagger \mathbf{S}_{\alpha'\alpha} a_{\lambda\alpha}. \quad (2.27)$$ CMFT(2.13)

2) **one-body Hamiltonian** for free particle:

$$\hat{H} = \int d^d r a^\dagger(\mathbf{r}) \left[\frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}) \right] a(\mathbf{r}) \tag{2.28}$$ CMFT(2.14)

with $\hat{\mathbf{p}} = -i\hbar\partial_x$.

3) The **local density operator** measuring particle density at certain point with coordinate $\mathbf{r}$:

$$\hat{\rho}(\mathbf{r}) = a^\dagger(\mathbf{r})a(\mathbf{r}). \tag{2.29}$$ CMFT(2.15)

4) The **total occupation number operator** is then $\hat{N} = \int d^d r a^\dagger(\mathbf{r})a(\mathbf{r})$ for continuous quantum numbers or $\hat{N} = \sum_\lambda a^\dagger_\lambda a_\lambda$ for discrete quantum numbers.

The next step is to consider **two-body operators** $\mathcal{O}_2$ needed to describe interactions. Classical case easy; quantum case complicated by indistinguishability.

Consider a symmetric pairwise interaction potential $V(\mathbf{r}_m, \mathbf{r}_n) = V(\mathbf{r}_n, \mathbf{r}_m)$. Let us search for an operator giving the expected outcome,

$$\hat{V}|\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N\rangle = \sum_{n<m}^{N} V(\mathbf{r}_n, \mathbf{r}_m)|\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N\rangle = \frac{1}{2}\sum_{n\neq m}^{N} V(\mathbf{r}_n, \mathbf{r}_m)|\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N\rangle. \tag{2.30}$$

One can guess the following form:

$$\hat{V} = \frac{1}{2}\int d^d r \int d^d r' a^\dagger(\mathbf{r})a^\dagger(\mathbf{r}')V(\mathbf{r}, \mathbf{r}')a(\mathbf{r}')a(\mathbf{r}). \tag{2.31}$$

That this is indeed the correct form can be checked by explicitly computing the action of the creation/annihilation operators on a generic state:

$$\begin{aligned}
&a^\dagger(\mathbf{r})a^\dagger(\mathbf{r}')a(\mathbf{r}')a(\mathbf{r})|\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N\rangle = a^\dagger(\mathbf{r})a^\dagger(\mathbf{r}')a(\mathbf{r}')a(\mathbf{r})a^\dagger(\mathbf{r}_1)...a^\dagger(\mathbf{r}_N)|0\rangle \\
&= \sum_{n=1}^{N} \zeta^{n-1}\delta(\mathbf{r}-\mathbf{r}_n)a^\dagger(\mathbf{r}_n)a^\dagger(\mathbf{r}')a(\mathbf{r}')a^\dagger(\mathbf{r}_1)...a^\dagger(\mathbf{r}_{n-1})a^\dagger(\mathbf{r}_{n+1})...a^\dagger(\mathbf{r}_N)|0\rangle \\
&= \sum_{n=1}^{N} \zeta^{n-1}\delta(\mathbf{r}-\mathbf{r}_n)\sum_{m\neq n}^{N} \delta(\mathbf{r}'-\mathbf{r}_m)a^\dagger(\mathbf{r}_n)a^\dagger(\mathbf{r}_1)...a^\dagger(\mathbf{r}_{n-1})a^\dagger(\mathbf{r}_{n+1})...a^\dagger(\mathbf{r}_N)|0\rangle \\
&= \sum_{n,m\neq n}^{N} \delta(\mathbf{r}-\mathbf{r}_n)\delta(\mathbf{r}'-\mathbf{r}_m)|\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N\rangle.
\end{aligned} \tag{2.32}$$

Note: the naive expression $\frac{1}{2}\int d^d r \int d^d r' V(\mathbf{r}, \mathbf{r}')\hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')$ does NOT work (exercise: show this). Referring to the logical structure (2.21), one must first *remove* the particles involved, weigh with the value of the operator matrix element, and then put the particles back in in the reverse order (to be consistent with the statistical signs under exchange).

The general expression for a two-body operator is thus

$$\mathcal{O}_2 = \sum_{\lambda\lambda'\mu\mu'} \mathcal{O}_{\mu\mu'\lambda\lambda'} a^\dagger_\mu a^\dagger_{\mu'} a_{\lambda'} a_\lambda, \qquad \mathcal{O}_{\mu\mu'\lambda\lambda'} = \langle \mu, \mu'|\mathcal{O}|\lambda\lambda'\rangle. \tag{2.33}$$ CMFT(2.16)

Examples 1) Coulomb interaction: just did it !

2) **spin-spin interaction** is fundamental in magnetism. From above:

$$\hat{V} = \frac{1}{2}\int d^d r \int d^d r' \sum_{\alpha\alpha'\beta\beta'} J(\mathbf{r},\mathbf{r}')\mathbf{S}_{\alpha\beta}\cdot\mathbf{S}_{\alpha'\beta'}a^\dagger_\alpha(\mathbf{r})a^\dagger_{\alpha'}(\mathbf{r}')a_{\beta'}(\mathbf{r}')a_\beta(\mathbf{r}), \tag{2.34}$$

with $J(\mathbf{r},\mathbf{r}')$ the exchange interaction (usually mediated in solids via electronic wavefunction overlap).

• More than 2-body interaction: not usually considered, look at literature.

Further in this chapter: develop fluency by considering specific examples, mostly the interacting electron gas in solid-state media.

2.2 Applications of operatorial quantization

Focus on electronic degrees of freedom. Principle 1: reduce many-body Hamiltonian to one containing only essential elements for electron dynamics. Include pure electron part H_e but also interactions between e and ion lattice. First approximation:

$$\hat{H}_0 = \int d^d r a^\dagger_\sigma(\mathbf{r}) \left[\frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r})\right] a_\sigma(\mathbf{r}),$$
$$\hat{V}_{ee} = \frac{1}{2}\int d^d r \int d^d r' V_{ee}(\mathbf{r}-\mathbf{r}') a^\dagger_\sigma(\mathbf{r}) a^\dagger_{\sigma'}(\mathbf{r}') a_{\sigma'}(\mathbf{r}') a_\sigma(\mathbf{r}), \tag{2.35}$$

with $V(\mathbf{r}) = \sum_I V_{ei}(\mathbf{R}_I - \mathbf{r})$ is the lattice potential felt by the electrons. We assume $\mathbf{R}_I$ fixed. Spin included for completeness.

Despite its simplicity, this accommodates a wide variety of phases from metals to insulators to magnets. To go further, we first study the non-interacting model.

Electrons in a periodic potential

Bloch's theorem: eigenstates in a periodic potential can be written as Bloch waves (see PRE:Phys A.2)

$$\psi_{\mathbf{k}n}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}n}(\mathbf{r}) \tag{2.36}$$

where the crystal momentum $\mathbf{k}$ takes values in first Brillouin zone $k_i \in [-\pi/a, \pi/a]$ (we assume that potential has same periodicity in all directions, $V(\mathbf{r} + a\mathbf{e}_i) = V(\mathbf{r})$).

n labels the energy bands of the solid, and $u_{\mathbf{k}n}(\mathbf{r}+a\mathbf{e}_i) = u_{\mathbf{k}n}(\mathbf{r})$ are purely periodic on the lattice.

Two complementary classes of materials where Bloch functions can be simplified considerably: nearly free systems, and tight-binding systems.

Nearly free electron systems Elemental metals from groups I-IV of periodic table: electrons are 'nearly free': their dynamics largely oblivious to Coulomb potential from ionic background and their mutual interactions. Conduction electrons experience a **pseudopotential** incorporating effects of ions and core electrons. Mobility so high that conduction electrons effectively screen their Coulomb interaction.

Good approx: neglect lattice potential (for crystal momenta away from boundaries of Brillouin zone $k_i = \pm\pi/a$). In practice: set Bloch function to unity, $u_{\mathbf{k}n} = 1$ and use plane waves as eigenstates of non-interacting Hamiltonian. Represent field operators in momentum space (CMFT(2.9) 2.20), with

$$\hat{H}_0 = \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2m} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} \tag{2.37}$$ CMFT(2.18)

with summation over all wavevectors $\mathbf{k}$ and summation over spin indices.

Turning on Coulomb between electrons:

$$\hat{V}_{ee} = \frac{1}{2L^d} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{ee}(\mathbf{q}) a^\dagger_{\mathbf{k}-\mathbf{q}\sigma} a^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} a_{\mathbf{k}'\sigma'} a_{\mathbf{k}\sigma} \tag{2.38}$$ CMFT(2.19)

where $V_{ee}(\mathbf{q}) = 4\pi e^2/q^2$ is the Fourier transform of Coulomb potential $V_{ee}(\mathbf{r}) = e^2/|\mathbf{r}|$ (we've set $4\pi\varepsilon = 1$).

Fourier transform of Coulomb potential

$$V(\mathbf{q}) = \int d^3r \frac{e^2}{|\mathbf{r}|} e^{i\mathbf{q}\cdot\mathbf{r}} = e^2 \int_0^\infty dr r^2 \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \frac{e^{iqr\cos\theta}}{r}$$
$$= 2\pi e^2 \int_0^\infty dr \frac{(-1)}{q} \int_{qr}^{-qr} dx e^{ix} \approx \frac{4\pi e^2}{q^2} i \int_0^\infty dx e^{-ix-\delta x} = \frac{4\pi e^2}{q^2} \tag{2.39}$$

where we have introduced a regulator δ.

NB: technical point: to ensure neutrality, we must take into account the positive charge of the ionic background. This is done by restricting the sum over $\mathbf{q}$ to a sum over $\mathbf{q} \neq 0$ (exercise).

$\hat{H}_0 + \hat{V}_{ee}$ is known as the **Jellium** model. The interaction term can be viewed as a scattering vertex between pairs of electrons.

Typical applications: need low energies. Zero-temperature ground state: one usually uses the noninteracting ground state as a basis.

Bohr's argument why this works: assume that the density of electron gas is such that each of the N particles occupies a volume of order a^d. Average kinetic energy per particle: $T \sim 1/ma^2$, while Coulomb potential scales as $V \sim e^2/a$. Thus, for a much smaller than the **Bohr radius** $a_0 = 1/e^2 m$, the interaction part is much smaller than the kinetic energy part. So: for the *dense* electron gas, the interaction energy can be treated as a perturbation. Most metals, however, have $a \sim a_0$, so the jellium model is not necessarily applicable to any particular case.

Ground state of system of N non-interacting particles: Pauli principle implies that all states with $\varepsilon_{\mathbf{k}} = \mathbf{k}^2/2m$ will be occupied up to a cutoff **Fermi energy** E_F.

Specifically, for system of size L, we have $\mathbf{k}$ with $k_i = 2\pi n_i/L$, $n_i \in \mathbb{Z}$. Summation extends to $|\mathbf{k}| < k_F$ with the **Fermi momentum** k_F defined through $k_F^2/2m = E_F$.

The ground state of noninteracting fermions is thus a **Fermi sphere**, whose volume is $\sim k_F^d$. Relation to occupation number: divide this by space volume per mode $(2\pi/L)^d$ so $N = C(k_F L)^d$ with C a dimensionless geometry-dependent constant (exercise: compute this for an arbitrary dimension d).

In the operatorial representation, the Fermi sea ground state is

$$|\Omega\rangle \equiv \mathcal{N} \prod_{|\mathbf{k}|<k_F,\sigma} a^\dagger_{\mathbf{k}\sigma}|0\rangle \tag{2.40}$$ CMFT(2.20)

with $|0\rangle$ the state with no electrons and $\mathcal{N}$ is a normalization constant. The particular order in which the product is taken has no physical meaning, but should really be set to a fixed convention in any particular calculation.

For weak interactions, low temperatures: physics governed by energetically low-lying excitations superimposed on state $|\Omega\rangle$. Therefore: declare Fermi sea $|\Omega\rangle$ to be the 'physical vacuum' of the theory. One can then consider a more physically meaningful set of creation/annihilation operators by introducing new operators $c, c^\dagger$ such that c now annihilate the Fermi sea itself,

$$c^\dagger_{\mathbf{k}\sigma} = \begin{cases} a^\dagger_{\mathbf{k}\sigma}, & k > k_F, \\ a_{\mathbf{k}\sigma}, & k \le k_F \end{cases} \qquad c_{\mathbf{k}\sigma} = \begin{cases} a_{\mathbf{k}\sigma}, & k > k_F, \\ a^\dagger_{\mathbf{k}\sigma}, & k \le k_F \end{cases} \tag{2.41}$$ CMFT(2.21)

Exercise: verify that $c_{\mathbf{k}\sigma}|\Omega\rangle = 0$ and that the CCR are preserved.

(2.37) + (2.38) represented in terms of (2.41) on vacuum (2.40) form the basis for the theory of *highly mobile* electron compounds.

Tight-binding systems Lattice potential presents a strong perturbation of conduction electrons. Realized in transition metal oxides. Picture: 'rarefied' lattice of ion cores: ions separated by distance much larger than Bohr radius of valence band electrons. In this '**atomic limit**', electrons are tightly bound to lattice centers. For microscopic theory: use a basis of **Wannier states** (see A.2), which are simply Fourier transforms of the Bloch states:

$$|\psi_{\mathbf{R}n}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in \mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{R}} |\psi_{\mathbf{k}n}\rangle, \qquad |\psi_{\mathbf{k}n}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |\psi_{\mathbf{R}n}\rangle. \tag{2.42}$$ CMFT(2.22)

The Wannier functions are peaked around the corresponding atomic site. Pure atomic limit: $\Psi_{\mathbf{R}n}(\mathbf{r})$ converges on nth orbital of atom centered on $\mathbf{R}$. Away from this limit: the N formerly degenerate states labeled by n split into an energy band.

Fermi energy between bands: **insulating** behavior. In a band: **metallic** behavior. Focus from now on on metallic case.

How to use Wannier states to simplify representation of (2.35) ? Notice that they form an orthonormal basis of single-particle Hilbert space: $|\mathbf{r}\rangle = \sum_{\mathbf{R}} |\psi_{\mathbf{R}}\rangle\langle\psi_{\mathbf{R}}|\mathbf{r}\rangle = \sum_{\mathbf{R}} \psi^*_{\mathbf{R}}(\mathbf{r})|\psi_{\mathbf{R}}\rangle$ (consider only $n = n_0$, drop band index). Thus: induces transformation

$$a^\dagger_\sigma(\mathbf{r}) = \sum_{\mathbf{R}} \psi^*_{\mathbf{R}}(\mathbf{r}) a^\dagger_{\mathbf{R}\sigma} \equiv \sum_i \psi^*_{\mathbf{R}_i}(\mathbf{r}) a^\dagger_{i\sigma} \tag{2.43}$$ CMFT(2.23)

between real and Wannier space operator basis ($i = 1, ..., N$ labels lattice sites).

Similarly, between Bloch and Wannier states:

$$a^\dagger_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i} a^\dagger_{i\sigma}, \qquad a^\dagger_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in \mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} a^\dagger_{\mathbf{k}\sigma}. \tag{2.44}$$ CMFT(2.24)

Can now use (2.43) and (2.44) to represent (2.35) with Wannier states (using the fact that Bloch states diagonalize single-particle terms):

$$\hat{H}_0 = \sum_{\mathbf{k}} \varepsilon_k a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} = \frac{1}{N} \sum_{ii'} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_{i'})} \varepsilon_k a^\dagger_{i\sigma} a_{i'\sigma} \equiv \sum_{ii'} a^\dagger_{i\sigma} t_{ii'} a_{i'\sigma}, \tag{2.45}$$ CMFT(2.24b)

with $t_{ii'} = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_{i'})} \varepsilon_k$.

→ electrons **hopping** from one lattice site $\mathbf{i}'$ to another $\mathbf{i}$. Strength of hopping matrix element $t_{ii'}$ controlled by effective overlap of neighbouring atoms' electronic wavefunctions. Tight-binding representation useful when orbital overlap is small, so only nearest neighbour hopping is important.

Exercise: 2D square lattice Set $t_{ii'} = -t$ for nearest neighbours. Hamiltonian:

$$\hat{H} = -t \sum_{i_x,i_y} \left[a^\dagger_{i_x+1,i_y} a_{i_x,i_y} + a^\dagger_{i_x,i_y+1} a_{i_x,i_y} + \text{h.c.} \right] \tag{2.46}$$

Basis of Fourier modes:

$$a_{i_x,i_y} = \frac{1}{\sqrt{N}} \sum_{k_x,k_y} e^{-iak_x i_x - iak_y i_y} a_{k_x,k_y} \tag{2.47}$$

with $N = N_x N_y$, $k_\alpha = \frac{2\pi}{aN_\alpha} n_\alpha$, $n_\alpha \in 0, 1, ..., N_\alpha - 1$. Hamiltonian becomes

$$\hat{H} = -2t \sum_{k_x,k_y} \left[\cos k_x a + \cos k_y a\right] a^\dagger_{k_x,k_y} a_{k_x,k_y}. \tag{2.48}$$

Constant energy: $-E/2t = \cos k_x a + \cos k_y a$. Half-filling: $k_y a = \pm(\pi - k_x a) \bmod 2\pi$ (square Fermi surface). Away from half-filling: around lowest energy, $E \simeq -2t(1 - k_x^2 a^2/2 + 1 - k_y^2 a^2/2 + ...) = -4t + ta^2(k_x^2 + k_y^2) + ...$, so Fermi surface is circular.

2.2.2 Interaction effects in the tight-binding system

Nearly free systems: Coulomb interaction can renormalize properties of systems, like effective masses, ..., but not really their nature. Electrons dressed by interactions become quasiparticles with the same quantum numbers (charge, spin) as free electrons. This concept forms the basis of Landau's Fermi liquid theory.

By contrast: in tight-binding systems, interactions can have a drastic effect and change nature of ground state and of the excitations. For example, we can then get a correlated magnetic state or insulating phase.

One sub-band; Wannier states, use (CMFT(2.23) 2.43) in Coulomb interaction (CMFT(2.17) 2.35):

$$\begin{aligned} \hat{V}_{ee} &= \sum_{ii'jj'} U_{ii'jj'} a^\dagger_{i\sigma} a^\dagger_{i'\sigma'} a_{j'\sigma'} a_{j\sigma} \\ U_{ii'jj'} &= \frac{1}{2} \int d^d r \int d^d r' \psi^*_{\mathbf{R}_i}(\mathbf{r}) \psi^*_{\mathbf{R}_{i'}}(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \psi_{\mathbf{R}_{j'}}(\mathbf{r}') \psi_{\mathbf{R}_j}(\mathbf{r}). \end{aligned} \tag{2.49}$$

With hopping, Hamiltonian becomes

$$\hat{H} = \sum_{ii'} a^\dagger_{i\sigma} t_{ii'} a_{i'\sigma} + \sum_{ii'jj'} U_{ii'jj'} a^\dagger_{i\sigma} a^\dagger_{i'\sigma'} a_{j'\sigma'} a_{j\sigma} \tag{2.50}$$

CMFT(2.27)

which is the **tight-binding representation** of the interaction Hamiltonian.

Most relevant terms: at most nearest neighbours. Three physically different classes of contributions:

• **Direct terms** $U_{ii'ii'} \equiv V_{ii'}$. Density fluctuations on neighbouring sites, $\sum_{i\neq i'} V_{ii'}\hat{n}_i\hat{n}_{i'}$ with $\hat{n}_i = \sum_\sigma a^\dagger_{i\sigma}a_{i\sigma}$. Can lead to global instabilities in charge distribution, *i.e. charge density wave* instabilities.

• **Exchange couplings** $U_{ii'jj'} \to U_{ijji}$ inducing magnetic correlations: set $J^F_{ij} \equiv U_{ijji}$. We have (using tensor notation $A\otimes B = \begin{pmatrix} A_{11}B & A_{12}B \\ A_{21}B & A_{22}B \end{pmatrix} = ...$)

$$\sigma^x\otimes\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\otimes\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

$$\sigma^y\otimes\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\otimes\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix},$$

$$\sigma^z\otimes\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\otimes\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\sigma\cdot\sigma = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = -\mathbf{1} + 2\mathbb{P} \tag{2.51}$$

where $\mathbb{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$ is the permutation operator matrix. In index notation,

$$\sigma_{\alpha\beta}\cdot\sigma_{\gamma\delta} = -\delta_{\alpha\beta}\delta_{\gamma\delta} + 2\delta_{\alpha\delta}\delta_{\beta\gamma} \tag{2.52}$$

so

$$\begin{aligned} :\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j: &:= \frac{1}{4}a^\dagger_{i\alpha}a^\dagger_{j\gamma}a_{j\delta}a_{i\beta}\times\sigma_{\alpha\beta}\cdot\sigma_{\gamma\delta} = -\frac{1}{4}a^\dagger_{i\alpha}a^\dagger_{j\gamma}a_{j\gamma}a_{i\alpha} + \frac{1}{2}a^\dagger_{i\alpha}a^\dagger_{j\beta}a_{j\alpha}a_{i\beta} \\ &= -\frac{1}{4}\hat{n}_i\hat{n}_j + \frac{1}{2}a^\dagger_{i\alpha}a^\dagger_{j\beta}a_{j\alpha}a_{i\beta} \end{aligned} \tag{2.53}$$

and therefore

$$a^\dagger_{i\alpha}a^\dagger_{j\beta}a_{i\beta}a_{j\alpha} = -2\left(:\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j: + \frac{1}{4}\hat{n}_i\hat{n}_j\right) \tag{2.54}$$

and

$$\sum_{i\neq j} U_{ijji}a^\dagger_{i\sigma}a^\dagger_{j\sigma'}a_{i\sigma'}a_{j\sigma} = -2\sum_{i\neq j} J^F_{ij}\left(\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j + \frac{1}{4}\hat{n}_i\hat{n}_j\right) \tag{2.55}$$

leading to **ferromagnetic coupling** of neighbouring spins. This comes from minimization of Coulomb interaction by minimizing overlap of wavefunctions: spins parallel mean total wavefunction antisymmetry requiring a node between the sites. Familiar from mechanism of **Hund's rule** in atomic physics.

Draw picture of overlapping wavefunctions. There must be a wavefunction node between sites for parallel spins, so Coulomb energy minimized.

• In far atomic limit: overalp of neighbouring orbitals small, t_{ij} and J^F_{ij} exponentially small in separation. On-site Coulomb **Hubbard interaction** $U_{iiii} \equiv U/2$, $\sum_{i\sigma\sigma'} U_{iiii} a^\dagger_{i\sigma} a^\dagger_{i\sigma'} a_{i\sigma'} a_{i\sigma} = \sum_i U \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ generates dominant interaction mechanism.

Keep only nearest neighbours, effective model becomes the **Hubbard model**

$$\hat{H} = -t \sum_{\langle ij \rangle} a^\dagger_{i\sigma} a_{j\sigma} + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \tag{2.56}$$

CMFT(2.28)

with standard notation for nearest neighbour.

Nobel prize-winning problem: solve the two-dimensional Hubbard model.

2.2.3 Mott-Hubbard transition and the magnetic state

Hubbard model: paradigm of strongly-correlated systems for over 4 decades. Ground state ? Excitations ??

Phase diagram: depends on a number of parameters. 1) ratio of Coulomb interaction scale to bandwidth U/t, 2) filling fraction n (average number of electrons per site), 3) (dimensionless) temperature T/t. Need only $0 \leq n \leq 1$ by particle-hole symmetry (exercise).

Look at low T, low density $n \ll 1$. Electrons hop around a lot. Expect metallic behaviour.

By contrast: consider half-filled case $n = 1$. If interactions are weak $U/t \ll 1$, may again expect metallic behaviour. On the other hand, for $U/t \gg 1$, double occupancy in inhibited and electrons become 'jammed'. In this strongly correlated state, mutual Coulomb interactions between electrons drives the system from a metallic to an insulating phase with properties very different from conventional band insulator.

Experimentally: low-T Mott insulator is usually accompanied by **antiferromagnetic ordering** of local moments. This can be understood from the Hubbard model (see the exercise 'Superexchange and antiferromagnetism'). By considering a half-filled lattice in the limit of large interactions $U \gg t$, one obtains an effective spin model with antiferromagnetic couplings,

$$\hat{H} = J\left(\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 - \frac{1}{4}\right) \tag{2.57}$$

with $J = 4\frac{t^2}{U}$ the **antiferromagnetic exchange** strength.

Interpretation: anti-parallel spins can take advantage of hybridization and reduce their kinetic energy by hopping to a neighbouring site. Pauli principle prevents parallel spins from doing this. This process, formulated by Anderson, is known as **superexchange**.

Extended lattice system: correlated magnetic insulator, with **Heisenberg Hamiltonian**

$$\hat{H} = J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n \tag{2.58}$$

CMFT(2.31)

with $J \sim t^2/U$. Charge degrees of freedom are quenched, spin DOF can propagate.

Doping away from half-filling: effective Hamiltonian is **t-J model**

$$\hat{H}_{t-J} = -t \sum_{\langle mn \rangle} \hat{P}_s a^\dagger_{m\sigma} a_{n\sigma} \hat{P}_s + J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n. \tag{2.59}$$

2.2.5 Quantum spin chains

Coulomb interaction: can lead either to ferromagnetic ('exchange') or antiferromagnetic ('superexchange') behaviour.

Models of localized quantum spins in one dimension: quantum spin chains.

Quantum ferromagnets Heisenberg model (1929):

$$\hat{H} = -J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n, \qquad J > 0. \tag{2.60}$$ CMFT(2.44)

Here, the spin can be carried by *e.g.* an atom with nonvanishing magnetic moment. All we need to know:

i) the lattice spin operators obey the $SU(2)$ algebra

$$\left[\hat{S}^i_m, \hat{S}^j_n\right] = i\delta_{mn}\varepsilon^{ijk}\hat{S}^k_n \tag{2.61}$$ CMFT(2.45)

ii) the total spin of each lattice site is S (half-integer).

Since $J > 0$, Hamiltonian favours configurations with spins parallel on adjacent sites. A ground state for the system: all spins in the same direction, say z, $|\Omega\rangle = \otimes_m |S_m\rangle$ where $|S_m\rangle$ is such that $S^z_m|S_m\rangle = S|S_m\rangle$.

System is in fact highly degenerate: rotating all spins the same way does not change the GSE, so system possesses a global rotation symmetry.

From before: expect that this global continuous symmetry will entail the presence of low-lying excitations. We now discuss these **spin waves**, starting from a semi-classical picture with $S >> 1$.

In limit of large S, and at low excitation energies, describe spins in terms of small fluctuations of the spins around their (ordered) expectation values.

Spin raising and lowering operators: $\hat{S}^{\pm}_m = \hat{S}^x_m \pm i\hat{S}^y_m$ with

$$\left[\hat{S}^z_m, \hat{S}^{\pm}_n\right] = \pm\delta_{nm}\hat{S}^{\pm}_m, \qquad \left[\hat{S}^+_m, \hat{S}^-_n\right] = 2\delta_{nm}S^z_m \tag{2.62}$$ CMFT(2.46)

To make use of fact that fluctuations are small, use **Holstein-Primakoff transformation**

$$\hat{S}^-_m = a^\dagger_m(2S - a^\dagger_m a_m)^{1/2}, \qquad \hat{S}^+_m = (2S - a^\dagger_m a_m)^{1/2}a_m, \qquad \hat{S}^z_m = S - a^\dagger_m a_m \tag{2.63}$$ CMFT(2.46a)

Utility: when $S \gg 1$, expand in powers of $1/S$ to get

$$\hat{S}^-_m \simeq (2S)^{1/2}a^\dagger_m, \qquad \hat{S}^+_m \simeq (2S)^{1/2}a_m, \qquad \hat{S}^z_m = S - a^\dagger_m a_m. \tag{2.64}$$

Substituting this in Heisenberg Hamiltonian, get

$$\begin{aligned}\hat{H} &= -J\sum_m \left(\hat{S}^z_m\hat{S}^z_{m+1} + \frac{1}{2}(\hat{S}^+_m\hat{S}^-_{m+1} + \hat{S}^-_m\hat{S}^+_{m+1})\right) \\ &= -JNS^2 - JS\sum_m \left(-2a^\dagger_m a_m + (a^\dagger_m a_{m+1} + \text{h.c.})\right) + O(S^0) \\ &= -JNS^2 + JS\sum_m (a^\dagger_{m+1} - a^\dagger_m)(a_{m+1} - a_m) + O(S^0)\end{aligned} \tag{2.65}$$

Keep only fluctuations to order S. Quadratic Hamiltonian: can be diagonalized by Fourier transform, imposing PBC $\hat{S}_{m+N} = \hat{S}_m$ for convenience,

$$a_k = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{ikm} a_m, \qquad a_m = \frac{1}{\sqrt{N}} \sum_{k \in BZ} e^{-ikm} a_k, \qquad [a_k, a_{k'}^\dagger] = \delta_{kk'} \tag{2.66}$$

Hamiltonian becomes

$$\hat{H} = -JNS^2 + \sum_{k \in BZ} \hbar\omega_k a_k^\dagger a_k + O(S^0), \qquad \hbar\omega_k = 2JS(1 - \cos k) = 4JS \sin^2(k/2) \tag{2.67}$$ CMFT(2.47)

For $k \to 0$, we have $\hbar\omega_k \to JSk^2$. These massless low-energy excitations are known as **magnons** and describe the spin-wave excitations of the ferromagnet. Higher order terms in $1/S$, if taken into account, then correspond to interactions between magnons.

Quantum antiferromagnets Antiferromagnetic Heisenberg model:

$$\hat{H} = J \sum_{\langle mn \rangle} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n, \qquad J > 0. \tag{2.68}$$ CMFT(2.44b)

Only a sign difference: physics radically altered !

For a **bipartite lattice** (two sublattices A, B such that neighbours of one sublattice always belong to other sublattice), the GS are close to a staggered configuration known as the **Néel state**, with all neighbouring spins antiparallel. Again, GS is degenerate.

For a non-bipartite lattice, *e.g.* the 2D triangular lattice, no spin arrangement can be found where all bonds can give full exchange contribution J. Such spin systems are called **frustrated**. Other example: **Kagomé lattice**.

Back to 1D: chain trivially bipartite. Strategy: express H in terms of bosonic operators. Before, for convenience: apply canonical transformation, rotating all spins on one sublattice by π around the x axis, *i.e.* $S_A \to \tilde{S}_A = S_A$, $S_B^x \to \tilde{S}_B^x = S_B^x$, $S_B^y \to \tilde{S}_B^y = -S_B^y$, $S_B^z \to \tilde{S}_B^z = -S_B^z$. Hamiltonian becomes

$$\hat{H} = -J \sum_m \left(\tilde{S}_m^z \tilde{S}_{m+1}^z - \frac{1}{2} (\tilde{S}_m^+ \tilde{S}_{m+1}^+ + \tilde{S}_m^- \tilde{S}_{m+1}^-) \right). \tag{2.69}$$

Doing Holstein-Primakoff, one gets

$$\hat{H} = -NJS^2 + JS \sum_m \left(a_m^\dagger a_m + a_{m+1}^\dagger a_{m+1} + a_m a_{m+1} + a_m^\dagger a_{m+1}^\dagger \right) + O(S^0) \tag{2.70}$$

Awkward structure: although quadratic, 'pairing'-like terms. After Fourier $a_m = \frac{1}{\sqrt{N}} \sum_k e^{-ikm} a_k$, get

$$\begin{aligned}
\hat{H} &= -NJS^2 + \frac{JS}{N} \sum_{k,k'} \left(\sum_m (e^{i(k-k')m} + e^{i(k-k')(m+1)}) a_k^\dagger a_{k'} + \right. \\
&\quad \left. + (\sum_m e^{-i(k+k')m - ik'}) a_k a_{k'} + (\sum_m e^{i(k+k')m + ik'}) a_k^\dagger a_{k'}^\dagger \right) \\
&= -NJS^2 + JS \sum_k \left(2a_k^\dagger a_k + e^{ik} a_k a_{-k} + e^{-ik} a_k^\dagger a_{-k}^\dagger \right) \\
&= -NJS^2 + JS \sum_k \left(2a_k^\dagger a_k + \cos k \; a_k a_{-k} + \cos k \; a_k^\dagger a_{-k}^\dagger \right) \\
&= -NJS^2 + JS \sum_k \left(a_k^\dagger a_k + a_{-k} a_{-k}^\dagger - 1 + \cos k (a_{-k} a_k + a_k^\dagger a_{-k}^\dagger) \right) \qquad (2.71)
\end{aligned}$$

where we have changed summation labels $k \to -k$ in some terms to simplify. This leads, finally, to

$$\hat{H} = -NJS(S+1) + JS \sum_k \begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} + O(S^0) \qquad (2.72)$$

with $\gamma_k = \cos k$.

To solve this: use a **Bogoliubov transformation**. This sort of transformation is extremely important for many applications, including superconductivity, so we do it in detail for the case at hand.

We look for a transformation from the set of operators a_k to new operators α_k preserving the canonical commutation relations

$$[\alpha_k, \alpha_{k'}^\dagger] = \delta_{kk'}. \qquad (2.73)$$

Writing the transformation explicitly in terms of a matrix U,

$$\begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} = \mathbf{U}^{-1} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix}, \qquad (2.74)$$

$$\begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} U_{11}(k) a_k + U_{12}(k) a_{-k}^\dagger \\ U_{21}(k) a_k + U_{22}(k) a_{-k}^\dagger \end{pmatrix} \qquad (2.75)$$

Consistency requires $U_{11}^*(-k) = U_{22}(k)$, $U_{12}^*(-k) = U_{21}(k)$. For preservation of the CCR, we thus need

$$\begin{aligned}
\delta_{kk'} = [\alpha_k, \alpha_{k'}^\dagger] &= \left[U_{11}(k) a_k + U_{12}(k) a_{-k}^\dagger, U_{21}(-k') a_{-k'} + U_{22}(-k') a_{k'}^\dagger \right] \\
&= (U_{11}(k) U_{22}(-k) - U_{12}(k) U_{21}(-k)) \delta_{kk'} = (|U_{11}(k)|^2 - |U_{12}(k)|^2) \delta_{kk'} \qquad (2.76)
\end{aligned}$$

We thus need to fix $|U_{11}(k)|^2 - |U_{12}(k)|^2 = 1$. A good representation for U is thus (we fix the phases here without loss of generality)

$$U = \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k \end{pmatrix} = \cosh\theta_k \mathbf{1} + \sinh\theta_k \sigma^x \qquad (2.77)$$

We have $U^\dagger = U$ but (by explicit calculation)

$$U^{-1} = \begin{pmatrix} \cosh\theta_k & -\sinh\theta_k \\ -\sinh\theta_k & \cosh\theta_k \end{pmatrix} = \cosh\theta_k \mathbf{1} - \sinh\theta_k \sigma^x = \sigma^z U \sigma^z. \tag{2.78}$$

Thus,

$$UU^{-1} = \mathbf{1} \to U\sigma^z U^\dagger \sigma^z = \mathbf{1} \to U\sigma^z U^\dagger = \sigma^z \tag{2.79}$$

this last condition being a **pseudo-unitarity** condition.

The quadratic form in our Hamiltonian is now

$$\begin{pmatrix} a_k^\dagger & a_{-k} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} \alpha_k^\dagger & \alpha_{-k} \end{pmatrix} (U_k^{-1})^\dagger (\mathbf{1} + \gamma_k \sigma^x) U_k^{-1} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix} \tag{2.80}$$

The matrix is

$$\begin{aligned} (U_k^{-1})^\dagger (\mathbf{1} + \gamma_k \sigma^x) U_k^{-1} &= \sigma^z U \sigma^z (\mathbf{1} + \gamma_k \sigma^x) \sigma^z U \sigma^z \\ &= (\cosh\theta \mathbf{1} - \sinh\theta \sigma^x)(\mathbf{1} + \gamma_k \sigma^x)(\cosh\theta \mathbf{1} - \sinh\theta \sigma^x) \\ &= \left[(\cosh\theta - \gamma\sinh\theta)\mathbf{1} + (-\sinh\theta + \gamma\cosh\theta)\sigma^x\right](\cosh\theta \mathbf{1} - \sinh\theta\sigma^x) \\ &= \left[\cosh\theta(\cosh\theta - \gamma\sinh\theta) - \sinh\theta(-\sinh\theta + \gamma\cosh\theta)\right]\mathbf{1} \\ &\quad + \left[\cosh\theta(-\sinh\theta + \gamma\cosh\theta) - \sinh\theta(\cosh\theta - \gamma\sinh\theta)\right]\sigma^x \\ &= \left[\cosh 2\theta - \gamma \sinh 2\theta\right]\mathbf{1} + \left[-\sinh 2\theta + \gamma\cosh 2\theta\right]\sigma^x \end{aligned} \tag{2.81}$$

where we have used the identities $\cosh^2\theta + \sinh^2\theta = \cosh 2\theta$, $2\sinh\theta\cosh\theta = \sinh 2\theta$.

The resulting matrix is thus diagonal if θ_k is chosen such that

$$\gamma_k = \tanh 2\theta_k \tag{2.82}$$

This makes

$$(U_k^{-1})^\dagger (\mathbf{1} + \gamma_k \sigma^x) U_k^{-1} = (\cosh 2\theta - \gamma \sinh 2\theta)\mathbf{1} = \frac{\cosh^2 2\theta - \sinh^2 2\theta}{\cosh 2\theta}\mathbf{1} = \frac{1}{\cosh 2\theta}\mathbf{1} \tag{2.83}$$

and since we have $1 - \gamma^2 = 1/\cosh^2 2\theta$ on the one hand, and $1 - \gamma^2 = 1 - \cos^2 k = \sin^2 k$ on the other, we finally find

$$\begin{pmatrix} \alpha_k^\dagger & \alpha_{-k} \end{pmatrix} (U_k^{-1})^\dagger (\mathbf{1} + \gamma_k \sigma^x) U_k^{-1} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix} = |\sin k| (\alpha_k^\dagger \alpha_k + \alpha_{-k}\alpha_{-k}^\dagger) \tag{2.84}$$

so the Hamiltonian is

$$\hat{H} = -NJS(S+1) + 2JS \sum_k |\sin k| \left(\alpha_k^\dagger \alpha_k + \frac{1}{2}\right) \tag{2.85}$$

CMFT(2.48)

For the antiferromagnet, the spin-wave excitations have a linear spectrum as $k \to 0$. Although derived for large S, this remains true even for $S = 1/2$, albeit with a renormalized velocity (linear coefficient).

The weakly-interacting Bose gas (Pitaevskii & Stringari, 4)

Ground-state energy and equation of state (Pitaevskii & Stringari, 4.1)

Hamiltonian for interacting BG:

$$\hat{H} = \sum_{\mathbf{k}} \frac{k^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{1}{2V} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}} a^\dagger_{\mathbf{k}'-\mathbf{q}} a_{\mathbf{k}'} a_{\mathbf{k}} \tag{2.86}$$ PS(4.5)

Simplification: only $\mathbf{q} = 0$ part of potential is important, so can write

$$\hat{H} = \sum_{\mathbf{k}} \frac{k^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{V_0}{2V} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}} a^\dagger_{\mathbf{k}'-\mathbf{q}} a_{\mathbf{k}'} a_{\mathbf{k}} \tag{2.87}$$ PS(4.7)

The idea here (Bogoliubov) is to exploit the fact that the ground state is macroscopically occupied, $\langle a^\dagger_0 a_0 \rangle = N_0 \sim O(N)$ to replace the quantum-mechanical operators $a_0, a^\dagger_0$ by c-numbers:

$$a_0 \equiv \sqrt{N_0} \tag{2.88}$$ PS(4.8)

in (2.87). In an ideal gas, at $T = 0$, $N_0 = N$. In an interacting gas, occupation numbers for states $\mathbf{k} \neq 0$ are finite but small. In a first approximation, we can thus neglect all $\mathbf{k} \neq 0$ operators in the Hamiltonian, and write the ground state energy as

$$E_0 = \frac{N^2 V_0}{2V} \tag{2.89}$$ PS(4.9)

Higher-order approximation: excitation spectrum and quantum fluctuations (Pitaevskii & Stringari 4.2)

Keeping only quadratic terms in $\mathbf{k} \neq 0$ operators, the Hamiltonian is

$$\hat{H} = \frac{V_0}{2V} a^\dagger_0 a^\dagger_0 a_0 a_0 + \sum_{\mathbf{k}} \frac{k^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{V_0}{2V} \sum_{\mathbf{k}\neq 0} (4 a^\dagger_0 a^\dagger_{\mathbf{k}} a_0 a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} a_0 a_0 + a^\dagger_0 a^\dagger_0 a_{\mathbf{k}} a_{-\mathbf{k}}). \tag{2.90}$$ PS(4.18)

Bogoliubov approximation: be careful with first term:

$$a^\dagger_0 a^\dagger_0 a_0 a_0 = N^2 - 2N \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}. \tag{2.91}$$ PS(4.19)

By defining the renormalized coupling g as

$$V_0 = g(1 + \frac{g}{V} \sum_{\mathbf{k}\neq 0} \frac{m}{k^2}), \tag{2.92}$$ SP(4.21)

the Hamiltonian becomes

$$\hat{H} = g\frac{N^2}{2V} + \sum_{\mathbf{k}} \frac{k^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{gn}{2} \sum_{\mathbf{k}\neq 0} \left(2 a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} + a_{\mathbf{k}} a_{-\mathbf{k}} + \frac{mgn}{k^2} \right) \tag{2.93}$$ PS(4.22)

This can be diagonalized using a Bogoliubov transformation, finally yielding

$$\hat{H} = E_0 + \sum_{\mathbf{k}} \varepsilon(k) b^\dagger_{\mathbf{k}} b_{\mathbf{k}}, \tag{2.94}$$ PS(4.29)

with ground state energy

$$E_0 = g\frac{N^2}{2V} + \frac{1}{2}\sum_{\mathbf{k}\neq 0}\left(\varepsilon(k) - gn - \frac{k^2}{2m} + \frac{m(gn)^2}{k^2}\right) \tag{2.95}$$ PS(4.30)

and excitation spectrum

$$\varepsilon(k) = \left[\frac{gn}{m}k^2 + (\frac{k^2}{2m})^2\right]^{1/2} \tag{2.96}$$ PS(4.31)

this being the famous **Bogoliubov dispersion relation** for the elementary excitations of the weakly interacting Bose gas.

Supplement: graphene and nanotubes

Two sublattices with base vectors $\mathbf{a}_1 = (\sqrt{3}/2, 1/2)a$ and $\mathbf{a}_2 = (\sqrt{3}/2, -1/2)a$. Tight-binding Hamiltonian:

$$\hat{H} = -t \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} (a_1^\dagger(\mathbf{r}) a_2(\mathbf{r}') + \text{h.c.}) + \varepsilon \sum_{\mathbf{r}} (a_1^\dagger(\mathbf{r}) a_1(\mathbf{r}) + a_2^\dagger(\mathbf{r}) a_2(\mathbf{r})) \tag{2.97}$$

Reciprocal lattice vectors: defined from $\mathbf{a}_i \mathbf{G}_j = 2\pi\delta_{ij}$. Get $\mathbf{G}_{1/2} = \frac{2\pi}{\sqrt{3}}(1, \pm\sqrt{3})$. Fourier decomposition of fields:

$$\begin{aligned} a_{a\sigma}(\mathbf{r}) &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\frac{a}{2\pi}(k_1\mathbf{G}_1 + k_2\mathbf{G}_2)\cdot\mathbf{r}} a_{a\sigma\mathbf{k}}, \\ a_{a\sigma\mathbf{k}} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\frac{a}{2\pi}(k_1\mathbf{G}_1 + k_2\mathbf{G}_2)\cdot\mathbf{r}} a_{a\sigma}(\mathbf{r}) \end{aligned} \tag{2.98}$$

with $k_i \in [0, 2\pi/a]$ quantized in units of $2\pi/L_i$ (N_i sites in direction i, N sites in total). Inversion formula:

$$\frac{1}{N} \sum_{\mathbf{r}} e^{i\frac{a}{2\pi}((k_1 - k_1')\mathbf{G}_1 + (k_2 - k_2')\mathbf{G}_2)\cdot\mathbf{r}} = \delta_{k_1 k_1'} \delta_{k_2 k_2'}. \tag{2.99}$$

In Hamiltonian: hopping term:

$$\begin{aligned} \hat{H}_{\text{hop}} &= -\frac{t}{N} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \sum_{\mathbf{k},\mathbf{k}'} e^{i\frac{a}{2\pi}(k_1\mathbf{G}_1 + k_2\mathbf{G}_2)\cdot\mathbf{r} - i\frac{a}{2\pi}(k_1'\mathbf{G}_1 + k_2'\mathbf{G}_2)\cdot\mathbf{r}'} a_{1\sigma\mathbf{k}}^\dagger a_{2\sigma\mathbf{k}'} + \text{h.c.} \\ &= -\frac{t}{N} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{r}} e^{-i\frac{a}{2\pi}((k_1\mathbf{G}_1 + k_2\mathbf{G}_2)\cdot\mathbf{r} - (k_1'\mathbf{G}_1 + k_2'\mathbf{G}_2)\cdot\mathbf{r})} \sum_{\alpha=1}^{3} e^{i\frac{a}{2\pi}(k_1\mathbf{G}_1 + k_2\mathbf{G}_2)\cdot\mathbf{b}_\alpha} a_{1\sigma\mathbf{k}}^\dagger a_{2\sigma\mathbf{k}'} + \text{h.c.} \\ &= -t \sum_{\mathbf{k}} (1 + e^{-ik_1 a} + e^{-i(k_1 - k_2)a}) a_{1\sigma\mathbf{k}}^\dagger a_{2\sigma\mathbf{k}} + \text{h.c.} \end{aligned} \tag{2.100}$$

Hoppings: $\mathbf{r} - \mathbf{r}' = \mathbf{b}_\alpha$, $\mathbf{b}_1 = 0$, $\mathbf{b}_2 = -\mathbf{a}_1$, $\mathbf{b}_3 = -\mathbf{a}_1 + \mathbf{a}_2$. We have $\mathbf{a}_1 \cdot \mathbf{G}_1 = 2\pi$, $\mathbf{a}_1 \cdot \mathbf{G}_2 = 0$, $\mathbf{a}_2 \cdot \mathbf{G}_1 = 0$, $\mathbf{a}_2 \cdot \mathbf{G}_2 = 2\pi$. Then, $\mathbf{G}_1 \cdot \mathbf{b}_2 = -2\pi$, $\mathbf{G}_2 \cdot \mathbf{b}_2 = 0$ and $\mathbf{G}_1 \cdot \mathbf{b}_3 = -2\pi$, $\mathbf{G}_2 \cdot \mathbf{b}_3 = 2\pi$.

Hamiltonian in Fourier modes:

$$\hat{H} = \sum_{\mathbf{k}\sigma} \begin{pmatrix} a_{1\sigma\mathbf{k}}^\dagger & a_{2\sigma\mathbf{k}}^\dagger \end{pmatrix} \begin{pmatrix} \varepsilon & -tf(\mathbf{k}) \\ -tf^*(\mathbf{k}) & \varepsilon \end{pmatrix} \begin{pmatrix} a_{1\sigma\mathbf{k}} \\ a_{2\sigma\mathbf{k}} \end{pmatrix} \tag{2.101}$$

with $f(\mathbf{k}) = 1 + e^{-ik_1 a} + e^{-i(k_1 - k_2)a}$.

Eigenvalues (for $\varepsilon = 0$):

$$\begin{aligned} \varepsilon_{\mathbf{k}} = \pm t |f(\mathbf{k})| &= \pm t \left[(1 + e^{-ik_1 a} + e^{-i(k_1 - k_2)a})(1 + e^{ik_1 a} + e^{i(k_1 - k_2)a}) \right]^{1/2} \\ &= \pm t \left[3 + 2\cos k_1 a + 2\cos(k_1 - k_2)a + 2\cos k_2 a \right]^{1/2}. \end{aligned} \tag{2.102}$$

We have $(k_x, k_y) = \frac{a}{2\pi}(k_1\mathbf{G}_1 + k_2\mathbf{G}_2) = (\frac{1}{\sqrt{3}}(k_1 + k_2), k_1 - k_2)$. The dispertion relation (2.102) vanishes for $k_1 = \frac{2\pi}{3a} = -k_2$ and $k_1 = -\frac{2\pi}{3a} = -k_2$, or $k_x = 0, k_y = \frac{4\pi}{3a}$ and $k_x = 0, k_y = -\frac{4\pi}{3a}$.

CMFT(2.25)

Carbon nanotube From graphene sheet: fold into armchair tube. Periodicity: $\psi(\mathbf{r}+N(\mathbf{a}_1+\mathbf{a}_2))=\psi(\mathbf{r})$ with N the number of cells in transverse direction, $L_\perp = N|\mathbf{a}_1+\mathbf{a}_2| = Na\sqrt{3}$ is tube circumference.

From Fourier representation of wavefunction: periodicity gives

$$e^{-\frac{a}{2\pi}(k_1\mathbf{G}_1+k_2\mathbf{G}_2)\cdot(\mathbf{a}_1+\mathbf{a}_2)N}=1, \tag{2.103}$$

so this gives quantization $k_1+k_2=\sqrt{3}k_x=2\pi m/Na=2\pi\sqrt{3}m/L_\perp$ with m integer.

Defining $k_\parallel = k_1-k_2=k_y$, dispersion relation becomes (for $k_1+k_2=0$, *i.e.* $m=0$)

$$\varepsilon_{k_\parallel} = \pm t\left[3+4\cos k_\parallel a/2+2\cos k_\parallel a\right]^{1/2} \tag{2.104}$$

This has nodes at points $k_\parallel a=\pm 4\pi/3$.

Chapter 3

Path integrals

PI

The objective of this chapter is to introduce the notion of path integrals, in other words 'sums over histories'. Although Feynman's name is most often associated with this framework, the original idea was first applied to stochastic processes and Brownian motion by N. Wiener, and then to quantum mechanics by P. A. M. Dirac. Feynman then considerably developed the quantum-mechanical framework during and right after his doctorate.

We will begin here by going back to the classical mechanics of a single particle performing random (Brownian) motion. Many important concepts are illustrated by solving this problem, including scaling, universality, divergences, regularization, renormalization, Green's functions and the fundamental equivalence of $d+1$-dimensional classical and d-dimensional quantum problems.

3.1 Classical wanderings

3.1.1 Brownian motion

Mankind has long been aware of the seemingly random motion of particles embedded within a fluid. For the historians among you, it might be interesting to remember that the Roman poet Lucretius described it in one of his scientific poems 'On the Nature of Things' (circa 60 BC). More importantly, it was qualitatively described in more scientific terms (through microscope observations) by Robert Brown in 1827. One of Albert Einstein's three famous papers of 1905 [2] is entirely devoted to precisely this subject, and helped establish Brownian motion as the definitive proof of the atomic hypothesis. Einstein was hereby able to determine the size of atoms, and Avogadro's number.

1905_Einstein_AP_322

We will here focus on a somewhat simplified scenario which tends to Brownian motion in a certain limit. This is the problem of a random walker on a regular lattice. Besides Brownian motion, the random walker problem has extremely many applications besides physics, for example in ecology, biology or economics.

3.1.2 The random walker

Our objective in this section will be limited to making some quantitative statements about random walks. Being by definition random, such a walk of course cannot be described exactly, and our objectives will thus be limited to making probabilistic statements.

We will begin by considering the most easily treatable case of a random walker moving in a d-dimensional hypercubic lattice. Let us thus consider d-dimensional Euclidean space, with basis

unit vectors

$$\hat{\boldsymbol{n}}_\mu, \qquad \mu = 1, ..., d, \qquad \text{such that} \qquad \hat{\boldsymbol{n}}_\mu \cdot \hat{\boldsymbol{n}}_\nu \equiv \sum_{i=1}^{d} \hat{\boldsymbol{n}}_\mu^i \hat{\boldsymbol{n}}_\nu^i = \delta_{\mu\nu}. \tag{3.1}$$

eq:dEbasisvec

Let us denote the lattice spacing as a. Our lattice is then defined by all points

$$\mathcal{L}_a \equiv \{\boldsymbol{r}\} \qquad \text{such that} \qquad \boldsymbol{r} = a \sum_{\mu=1}^{d} n^\mu \hat{\boldsymbol{n}}_\mu, \qquad n^\mu \in \mathbb{N}. \tag{3.2}$$

Each point has $2d$ neighbours; this is known as the **coordination number** of this lattice, and we will denote it as $c_{\mathcal{L}_a}$.

Let us now imagine that we are observing a walker obeying the following rules:[1]

- **rule 1**: at each time interval δt, the walker takes one step on the lattice;
- **rule 2**: the direction each step is taken in, is uniformly distributed between the $c_{\mathcal{L}_a}$ possible choices.

Examples of paths traced out by such a walker are provided in Fig. 3.1 for the case of a two-dimensional square lattice. Some comments are immediately in order. The meanderings of the walker away from the origin are slow: some sites are visited many times over (the number of times a site is visited is not visible in the plots, but can be imagined) and the path therefore tends to be divided into dense clusters where the wanderer keeps retracing his steps, linked by narrow bridges representing rarer chance instances where the wanderer follows more or less one direction for a while. Very occasionally, the walker wanders much further, as if a drift current was present (*e.g.* the bottom right instance of Fig. 3.1). These instances are rare events.

fig:randomwalk1

fig:randomwalk1

The second rule is an expression of the **Markov property** of the random walk, namely that the status of the system at a point in time is sufficient to determine its status at the next time increment. Processes with discrete time evolution obeying the Markov property are commonly referred to as **Markov chains.**

The random walker, despite following extremely simple rules, displays rather interesting behaviour (you can view this as an example of **emergence**: simple rules yield rich physics). We can ask ourselves very many questions about the walker. Most fundamental of all is:

- What is the conditional probability $P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0}$ of finding the walker at site $\boldsymbol{r}_1$ at time $t_1 = t_0 + s\delta t$ (s being the number of steps taken) given that it was at $\boldsymbol{r}_0$ at time t_0?

This probability only makes sense if $t_1 \geq t_0$[2]. In theory, a detailed answer to this question is sufficient to answer all possible questions one might have about the random walker, since these will be expressible as functions of the $P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0}$.

We can state a few obvious facts. We consider a (spatial *and* time) translationally-invariant system, so the probabilities are unchanged by a constant shift of coordinates:

$$P_{\boldsymbol{r}_1-\boldsymbol{r}_2,t_1|\boldsymbol{r}_0-\boldsymbol{r}_2,t_0} = P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = P_{\boldsymbol{r}_1,t_1+t_2|\boldsymbol{r}_0,t_0+t_2}. \tag{3.3}$$

We can therefore view the origins $\boldsymbol{r}_0$, t_0 as being fixed from now on. By definition, at time t_0, our walker is standing at $\boldsymbol{r}_0$:

$$P_{\boldsymbol{r}_1,t_0|\boldsymbol{r}_0,t_0} = \delta_{\boldsymbol{r}_1,\boldsymbol{r}_0}. \tag{3.4}$$

[1] The commonly made analogy to a drunken wanderer is entirely inappropriate: our walker is a very predictable being, since it *certainly* makes one step at each unit of time with *perfectly uniformly random* choice of direction.

[2] You can view this as a manifestation of the 'arrow of time' in classical mechanics. In quantum mechanics, we will be able to make sense of propagators for negative times.

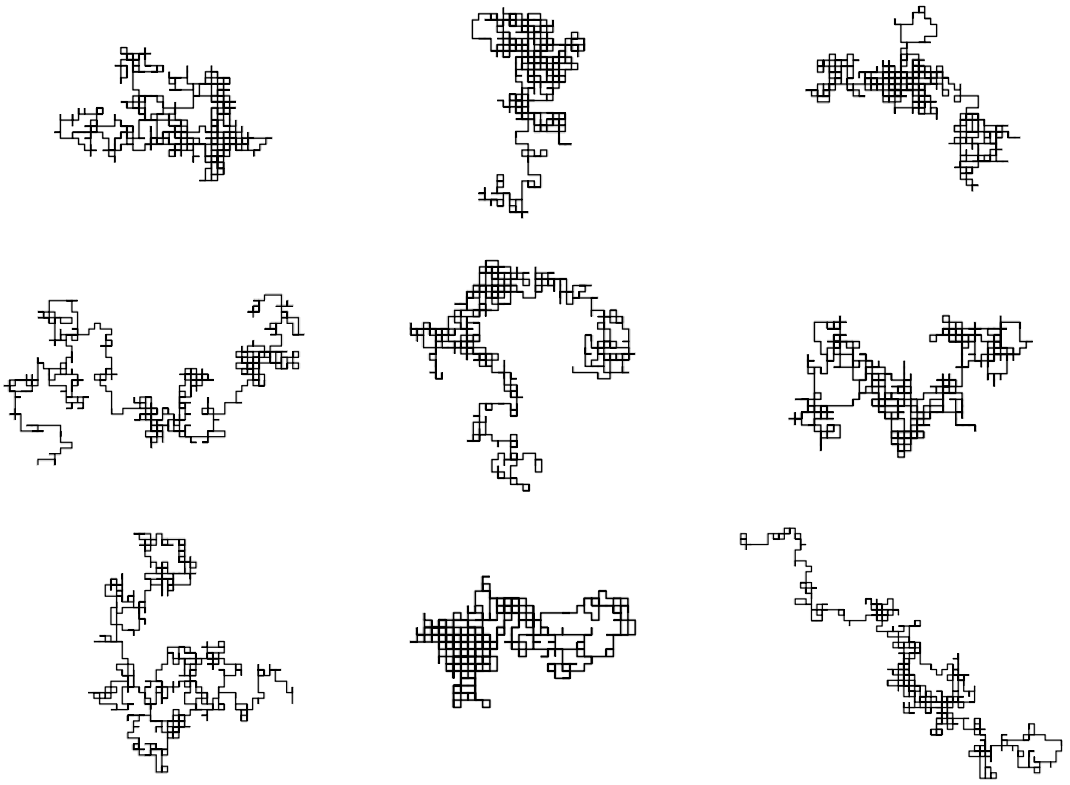

Figure 3.1: Examples of random walks on the square lattice. Each walk consists of 1000 steps. fig:randomwalk1

Second, all probabilities are positive-definite and bounded:

$$0 \leq P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} \leq 1 \quad \forall\, \boldsymbol{r}_1, \quad \forall\, t_1 \geq t_0. \tag{3.5}$$

Third, the walker must be *somewhere*, so the probabilities obey the 'sum rule'

$$\sum_{\boldsymbol{r}_1 \in \mathcal{L}_a} P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = 1 \quad \forall\, t_1 \geq t_0. \tag{3.6}$$

There are some further obvious facts that can be stated. For example, the probability must vanish if the time is not sufficient to go from $\boldsymbol{r}_0$ to $\boldsymbol{r}_1$ in time $t_1 - t_0$:

$$P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = 0 \quad \text{if} \quad |\boldsymbol{r}_1 - \boldsymbol{r}_0| > \frac{a}{\delta t}(t_1 - t_0) \tag{3.7}$$

(meaning that we can interpret $a/\delta t \equiv v_{\max}$ as an effective maximal (light) velocity), so the time dynamics in our system is causal: the walker will not be nonlocally teleported around the lattice under time evolution. As we will see, this effective light velocity is not very meaningful: the overwhelming majority of random walks will propagate at a diffusion velocity $v_d \ll v_{\max}$.

Another statement one could make is that since our hypercubic lattice is bipartite[3], the probability possesses a 'parity' feature whereby it is alternately (non)vanishing on each sublattice.

[3]That is: it can be divided into two sublattices A and B such that all nearest neighbours of $\boldsymbol{r} \in A$ are in B, and vice-versa.

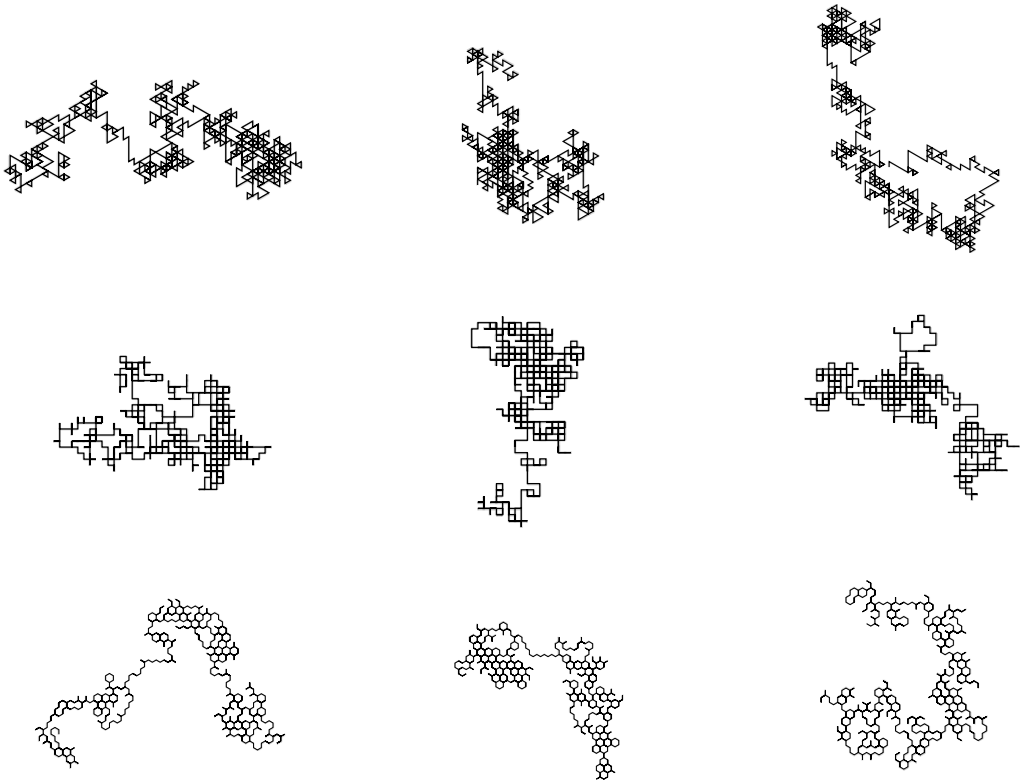

Figure 3.2: Examples of random walks on the triangular (top), square (middle) and honeycomb (bottom) lattices. Each walk consists of 1000 steps. The similarity between these three instances is an illustration of the concept of universality. fig:randomwal

This is an example of a **non-universal** statement: it relies on the microscopic features of the lattice here considered, and will not be true of other lattices. The most appealing way of thinking which we will pursue focuses of course on the universal features. What is meant by this? Things that do *not* depend on microscopic details, but rather apply to whole classes of situations. As a simple illustration here, consider the problem of the random walker but on different lattices, say the triangular and honeycomb ones. The triangular lattice is not bipartite; the honeycomb one is. Looking at Fig. fig:randomwalk2 3.2, in which example paths are given for triangular, square and honeycomb lattices, one can observe a rather striking similarity. This similarity becomes exact in the so-called **scaling limit** taking the time interval (number of steps) and distance scale (lattice spacing) respectively to ∞ and zero in a meaningful way (which we will do later for the square lattice). The concept of scaling is illustrated in Fig. fig:randomwalkscaling 3.3.

3.1.2.1 Time evolution

Let us now focus on the time dependence of the occupation probabilities. Our starting point is the implementation of the second rule of the walker, namely the one-time-step relation

$$P_{\boldsymbol{r}_1,t_1+\delta t|\boldsymbol{r}_0,t_0} = \frac{1}{c_{\mathcal{L}_a}} \sum_{\boldsymbol{r}'\text{n.n.}\boldsymbol{r}_1} P_{\boldsymbol{r}',t_1|\boldsymbol{r}_0,t_0} \tag{3.8}$$

Figure 3.3: Illustration of scaling in random walks. The top left walk has 125 steps of length 32 on the two-dimensional square lattice. Each subsequent curve has four times as many steps of half the length. The mean distance from the origin reached by the walker remains the same. fig:randomwalkscaling

where we write the requirement that $\boldsymbol{r}'$ be nearest neighbour to $\boldsymbol{r}_1$ as $\boldsymbol{r}'_{\text{n.n.}}\boldsymbol{r}_1$. For our hypercubic lattice, this is specialized to

$$P_{\boldsymbol{r}_1,t_1+\delta t|\boldsymbol{r}_0,t_0} = \frac{1}{2d}\sum_{\sigma=\pm 1}\sum_{\mu=1}^{d} P_{\boldsymbol{r}_1+a\sigma\hat{\boldsymbol{n}}_\mu,t_1|\boldsymbol{r}_0,t_0}. \tag{3.9}$$ eq:onetimestepcubic

We here recognize the discretized version of the Laplacian operator, which we will denote ∇_a^2 and define as

$$\nabla_a^2 f_{\boldsymbol{r}} \equiv \frac{1}{a^2}\sum_{\mu=1}^{d}\left[f_{\boldsymbol{r}+a\hat{\boldsymbol{n}}_\mu} + f_{\boldsymbol{r}-a\hat{\boldsymbol{n}}_\mu} - 2f_{\boldsymbol{r}}\right]. \tag{3.10}$$

This scales to the usual Laplacian in the continuum limit: if the lattice-defined $f_{\boldsymbol{r}}$ scales to a differentiable function $f(\boldsymbol{r})$, then

$$\lim_{a\to 0}\nabla_a^2 f_{\boldsymbol{r}} = \nabla^2 f(\boldsymbol{r}). \tag{3.11}$$

We can thus rewrite our one-time-step relation as

$$P_{\boldsymbol{r}_1,t_1+\delta t|\boldsymbol{r}_0,t_0} - P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = \frac{a^2}{2d}\nabla_a^2 P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0}. \tag{3.12}$$ eq:onetimestep

This is simply a lattice version of the continuum diffusion equation (in reality here: the heat equation)

$$\left(\frac{\partial}{\partial t} - D\,\nabla^2\right)P(\boldsymbol{r},t) = 0, \tag{3.13}$$

in which D (the **diffusion constant**) parametrizes the efficiency of the diffusion (the higher D is, the quicker an initial state diffuses). Here, this constant is taken as the limiting value

(assumed to be finite, and thus choosing $a^2 \propto \delta t$ in the scaling limit)

$$D = \lim_{\substack{a\to 0\\ \delta t\to 0}} \frac{a^2}{2d\delta t}. \tag{3.14}$$ eq:Dsq

Getting back to our problem of describing the random walker, given an initial configuration of probabilities

$$P_{\boldsymbol{r},t_0|\boldsymbol{r}_0,t_0} \equiv P_{\boldsymbol{r},t_0}, \tag{3.15}$$

the probability configuration at all times $t_1 > t_0$ is thus obtainable from the solution of (3.12), eq:onetimestep which can in turn easily be obtained by simple Fourier transformation. Adopting the convention

$$f_{\boldsymbol{r}} = a^d \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d\boldsymbol{k}}{(2\pi)^d} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} f(\boldsymbol{k}), \qquad f(\boldsymbol{k}) = \sum_{\boldsymbol{r}\in\mathcal{L}_a} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} f_{\boldsymbol{r}}, \tag{3.16}$$

we can write our single-site-localized initial condition as

$$P_{\boldsymbol{r},t_0|\boldsymbol{r}_0,t_0} = \delta_{\boldsymbol{r},\boldsymbol{r}_0}, \qquad P_{\boldsymbol{k},t_0|\boldsymbol{r}_0,t_0} = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_0}. \tag{3.17}$$

The one-time-step equation (3.12) eq:onetimestep becomes

$$P_{\boldsymbol{k},t_1+\delta t|\boldsymbol{r}_0,t_0} = \frac{1}{d}\sum_{\mu=1}^{d} \cos(k^\mu a)\ P_{\boldsymbol{k},t_1|\boldsymbol{r}_0,t_0}. \tag{3.18}$$

Using this, we can immediately solve (3.12) eq:onetimestep for arbitrary $t_1 \geq t_0$ as

$$P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = a^d \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d\boldsymbol{k}}{(2\pi)^d} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_0)} \left[\frac{1}{d}\sum_{\mu=1}^{d}\cos(k^\mu a)\right]^{\frac{t_1-t_0}{\delta t}}. \tag{3.19}$$ eq:onetimeste

This is the full, exact solution of our problem: no approximations have been made, so this equation is exact for all values of $\boldsymbol{r}_1$ and $t_1 \geq t_0$. In particular, the fact that all probabilities are positive can be easily verified.

This is all very nice, but the fact remains that (3.19) eq:onetimestepsolved is a bit unwieldy and does not make the physics very transparent. The question thus now becomes: can this equation be further simplified, at least for the most likely paths that our walker can follow?

3.1.2.2 Continuum limit

Let us consider taking the limit $\delta t \to 0$. For a fixed time interval $t_1 - t_0$, the exponent of the square bracket in (3.19) eq:Onetimestepsolved becomes very large. This term would only survive in the limit $\delta t \to 0$ if we were to simultaneously scale $k^\mu a$ to zero. For finite momenta, this means taking the lattice spacing to zero (which justifies calling what we are doing here a 'continuum limit'). Expanding the cosine under this assumption gives

$$\left[\frac{1}{d}\sum_{\mu=1}^{d}\cos(k^\mu a)\right]^{\frac{t_1-t_0}{\delta t}} = \left[1 - \frac{a^2}{2d}\boldsymbol{k}^2 + ...\right]^{\frac{t_1-t_0}{\delta t}} \to e^{-(t_1-t_0)\frac{a^2}{2d\delta t}\boldsymbol{k}^2} \tag{3.20}$$

in which we now explicitly recognize our diffusion constant D (3.14). eq:Dsq In this limit, the probability density (per unit volume) of finding the particle around $\boldsymbol{r}_1$ at time t_1 scales to a smooth function

of space and time coordinates:

$$p(\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0)\equiv\lim a^{-d}P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0}=\int_{-\infty}^{\infty}\frac{d^d\boldsymbol{k}}{(2\pi)^d}e^{-(t_1-t_0)D\boldsymbol{k}^2+i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_0)}$$
$$=\frac{1}{[4\pi D(t_1-t_0)]^{\frac{d}{2}}}\exp\left[-\frac{|\boldsymbol{r}_1-\boldsymbol{r}_0|^2}{4D(t_1-t_0)}\right]. \tag{3.21}$$

From this equation, we immediately see that after a time interval t_1-t_0, the typical distance from the origin at which we find our walker is

$$|\boldsymbol{r}_1-\boldsymbol{r}_0|\sim(t_1-t_0)^{\nu},\qquad \nu=\frac{1}{2}. \tag{3.22}$$

This is our first example of a **critical exponent**. Here, it is the **Hausdorff dimension** of the curve: the path has total length $\sim t_1-t_0$, but it is confined in a ball of radius $\sim(t_1-t_0)^{\frac{1}{2}}$.

Summarizing, this probability density is a positive-definite symmetric kernel which satisfies the normalization condition

$$\int d^d\boldsymbol{r}\ p(\boldsymbol{r},t|\boldsymbol{r}_0,t_0)=1, \tag{3.23}$$

and the diffusion equation

$$\left(\frac{\partial}{\partial t}-D\nabla^2\right)p(\boldsymbol{r},t|\boldsymbol{r}_0,t_0)=0 \tag{3.24}$$ eq:diffusion

with initial condition

$$p(\boldsymbol{r}_1,t_0|\boldsymbol{r}_0,t_0)=\delta^{(d)}(\boldsymbol{r}_1-\boldsymbol{r}_0). \tag{3.25}$$

Another interesting equation obeyed by the kernel originates from the fact that at any intermediate time, the walker must be somewhere. This completely trivial statement translates into the following nontrivial composition property

$$\int d^d\boldsymbol{r}_1\ p(\boldsymbol{r}_2,t_2|\boldsymbol{r}_1,t_1)\ p(\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0)=p(\boldsymbol{r}_2,t_2|\boldsymbol{r}_0,t_0),\qquad\forall\ t_1\text{ such that }t_2>t_1>t_0. \tag{3.26}$$ eq:pcomposition

Said otherwise, our walker has no memory whatsoever. The diffusion process is purely local in time (in other words: there are no retarded effects), as per the (microscopic) Markovian dynamics highlighted previously.

3.1.2.3 Green's function

A simple question we can now ask (and answer!) is the following: how much time does our walker spend on a given point $\boldsymbol{r}_1$? This is simply given by explicitly summing (3.19) eq:onetimestepsolved

$$\sum_{n=0}^{\infty}P_{\boldsymbol{r}_1,t_0+n\delta t|\boldsymbol{r}_0,t_0}=a^d\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}}\frac{d^d\boldsymbol{k}}{(2\pi)^d}\frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_0)}}{1-\frac{1}{d}\sum_{\mu=1}^{d}\cos(k^\mu a)}\equiv\mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0}. \tag{3.27}$$ eq:Gsqlat

As can directly be seen from (3.9), this quantity obeys the equation eq:onetimestepcubic

$$\mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0}=\delta_{\boldsymbol{r}_1,\boldsymbol{r}_0}+\frac{1}{2d}\sum_{\mu=1}^{d}\left[\mathcal{G}_{\boldsymbol{r}_1+a\hat{\boldsymbol{n}}_\mu-\boldsymbol{r}_0}+\mathcal{G}_{\boldsymbol{r}_1-a\hat{\boldsymbol{n}}_\mu-\boldsymbol{r}_0}\right] \tag{3.28}$$

or more economically in terms of our lattice Laplacian

$$-\nabla_a^2\mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0}=\frac{2d}{a^2}\delta_{\boldsymbol{r}_1,\boldsymbol{r}_0}. \tag{3.29}$$ eq:GreensdiscreteLap

The kernel $\mathcal{G}$ is thus the **Green's function** of (a constant times) the Laplacian, namely it is the kernel which inverts this operator[4]. The physical interpretation of the Green's function is thus quite direct for our random walker: for an infinitely long walk, $\mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0}$ is the total number of time steps spent by our walker at $\boldsymbol{r}_1$, given that it started at $\boldsymbol{r}_0$.

3.1.2.4 Divergences

Simply by looking at the integral representation (3.27) in the region of small momenta, we see that the Green's function is given by a convergent integral for $d > 2$. For $d = 2$, we see that we get a logarithmic divergence (in terms of a smallest allowable wavelength/infrared cutoff $k_{\min}$ which we would like to put identically to zero) of the form $\int \frac{d^2\boldsymbol{k}}{k^2} \sim -\ln k_{\min}$; the $d = 1$ case diverges like $1/k_{\min}$. This is simply a manifestation of the fact that in $d \leq 2$, the walker left to wander for an infinite time, will tend to spend an infinite amount of time at each point of the lattice.

Infinities make the interpretation of our results problematic, and we must find a way to deal with them. You will no doubt have heard that dealing with infinities is the main object of the theory of **renormalization**. Handling the simple infinities we encounter here can thus be seen as a warm-up for more advanced dealings with renormalization.

Subtraction. The first way to deal with infinities is to... get rid of them by subtracting them away. This is not as mindless as it may seem. Note first that, as a function of position, the total time spent in one point is maximal at the origin. In other words, our Green's function $\mathcal{G}$ is maximal at $\boldsymbol{r}_1 = \boldsymbol{r}_0$. We can thus consider a Green's function $\mathcal{G}^s$ (s for *subtracted*) which is finite for all d by simply subtracting the (d-dependent, possibly infinity) constant $\mathcal{G}_{\boldsymbol{0}}$:

$$\mathcal{G}^s_{\boldsymbol{r}_1-\boldsymbol{r}_0} = \mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0} - \mathcal{G}_{\boldsymbol{0}} = a^d \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d\boldsymbol{k}}{(2\pi)^d} \frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_0)} - 1}{1 - \frac{1}{d}\sum_{\mu=1}^{d} \cos(k^\mu a)}. \tag{3.30}$$

Since we have merely subtracted a constant, this new kernel still obeys (3.29), but it is not positive definite anymore. If fact, it is now *negative definite*.

Exercise: Green's function in one dimension. Show that the subtracted Green's function in one dimension is exactly given by

$$\mathcal{G}^s_{\boldsymbol{r}_1-\boldsymbol{r}_0} = -\frac{|\boldsymbol{r}_1 - \boldsymbol{r}_0|}{a}. \tag{3.31}$$

Derivation:

$$\mathcal{G}^s_r = a \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} \frac{e^{ikr} - 1}{1 - \cos ka} = -a \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} \frac{\sin^2 \frac{kr}{2}}{\sin^2 \frac{ka}{2}} \overset{\text{[GR] } 3.624.6}{=} -\frac{r}{a}.$$

Regularization. Another way of dealing with infinities is to introduce some sort of deformation parameter in the theory which renders all sums or integrals finite. Here, the infinities came from the fact that we are considering an infinitely long duration of the walk, our walker never getting tired of hopping around. Let us thus add assume that our walker obeys the additional rule, to be enforced with **rule 1** and **rule 2**:

[4] The Green's function of an operator is of course only defined modulo a function which is in the null space of this operator. Consider here adding a (lattice) harmonic function $f_h(\boldsymbol{r})$ such that $\nabla_a^2 f_h = 0$.

- **rule 3**: during each time step, with probability η, our walker gets exhausted, quits the game and disappears from the lattice.

A more physical interpretation of this 'exhaustible walker' problem is for example to imagine that our walker is a radioactive particle subject to decay.

Given such a finite probability of our walker disappearing at each time step, our probabilities (now denoted by a superscript η) are now simply given by a time-dependent rescaling of our earlier solution

$$P^{(\eta)}_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = (1-\eta)^{\frac{t_1-t_0}{\delta t}} P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0}. \tag{3.32}$$

eq:Pexhaustible

Note that the sum rule now becomes

$$\sum_{\boldsymbol{r}_1} P^{(\eta)}_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = (1-\eta)^{\frac{t_1-t_0}{\delta t}} \qquad \forall\ t_1 \geq t_0. \tag{3.33}$$

For this exhaustible walker, the Green's function becomes

$$\mathcal{G}^{(\eta)}_{\boldsymbol{r}_1-\boldsymbol{r}_0} \equiv \sum_{n=0}^{\infty} (1-\eta)^n P_{\boldsymbol{r}_1,t_0+n\delta t|\boldsymbol{r}_0,t_0}. \tag{3.34}$$

We obviously have that our earlier Green's function is given by the limit $\eta \to 0$ of the exhaustible walker Green's function:

$$\mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0} = \lim_{\eta\to 0} \mathcal{G}^{(\eta)}_{\boldsymbol{r}_1-\boldsymbol{r}_0}. \tag{3.35}$$

Now however, the integral representation for $\mathcal{G}^{(\eta)}$ converges for all $\eta > 0$ (we by definition necessarily have $0 \leq \eta \leq 1$). This representation is

$$\mathcal{G}^{(\eta)}_{\boldsymbol{r}_1-\boldsymbol{r}_0} = \frac{a^d}{1-\eta} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d\boldsymbol{k}}{(2\pi)^d} \frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_0)}}{\frac{1}{1-\eta} - \frac{1}{d}\sum_{\mu=1}^{d}\cos(k^\mu a)} \tag{3.36}$$

and obeys the equation

$$\left[-\nabla_a^2 + m^2\right] \mathcal{G}^{(m)}_{\boldsymbol{r}_1-\boldsymbol{r}_0} = \frac{2d}{a^2(1-\eta)} \delta_{\boldsymbol{r}_1,\boldsymbol{r}_0} \tag{3.37}$$

where m can be interpreted as the **effective mass** (note that we now use the mass as superscript label for the Green's function). This is given here by

$$m^2 \equiv \frac{2d}{a^2} \frac{\eta}{1-\eta} \tag{3.38}$$

(which is indeed a positive quantity since $0 \leq \eta \leq 1$) For our walker, the mass is thus related to the rate of exhaustion our walker displays as he wanders.

In the scaling limit, we will also take the mass to be finite (this means that we should scale $\eta \sim a^2 \sim \delta t$). The proper scaling of the Green's function is

$$\mathcal{G}_m(\boldsymbol{r}) \equiv \lim \frac{1}{2da^{d-2}} \mathcal{G}^{(m)}_{\boldsymbol{r}} = \int_{-\infty}^{+\infty} \frac{d^d\boldsymbol{k}}{(2\pi)^d} \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{\boldsymbol{k}^2 + m^2} \tag{3.39}$$

eq:Gm

this function obeying the equation

$$\left[-\nabla^2 + m^2\right] \mathcal{G}_m(\boldsymbol{r} - \boldsymbol{r}_0) = \delta(\boldsymbol{r} - \boldsymbol{r}_0), \qquad \boldsymbol{r} \in \mathbb{R}^d. \tag{3.40}$$

Exercise: massive Green's functions in $d = 1, 2, 3$.

a) Show that the 1d Green's function is

$$\mathcal{G}_m(r) = \frac{e^{-m|r|}}{2m} \tag{3.41}$$ eq:Gm1d

so the correlation decays with distance on a scale given by the correlation length $\xi = 1/m$.

b) show that in the 2d case, the Green's function becomes

$$\mathcal{G}_m(\boldsymbol{r})|_{d=2} = \int \frac{d^2k}{(2\pi)^2} \frac{e^{-i\mathbf{k}\cdot\boldsymbol{r}}}{k^2+m^2} = \frac{1}{2\pi} K_0(m|\boldsymbol{r}|) \tag{3.42}$$ eq:Gm2d

(where K_0 is the modified Bessel function of the second kind), with limits

$$\mathcal{G}_m(\boldsymbol{r})|_{d=2} \simeq -\frac{1}{2\pi} \ln[\frac{m}{2}|\boldsymbol{r}|], \qquad |\boldsymbol{r}| \ll 1/m \tag{3.43}$$

and

$$\mathcal{G}_m(\boldsymbol{r})|_{d=2} \simeq \frac{1}{2}(2\pi m|\boldsymbol{r}|)^{-1/2} e^{-m|\boldsymbol{r}|}, \qquad |\boldsymbol{r}| \gg 1/m. \tag{3.44}$$

c) show that in the 3d case, we get

$$\mathcal{G}_m(\boldsymbol{r})|_{d=3} = \int \frac{d^3k}{(2\pi)^3} \frac{e^{-i\mathbf{k}\cdot\boldsymbol{r}}}{k^2+m^2} = \frac{e^{-m|\boldsymbol{r}|}}{4\pi|\boldsymbol{r}|}. \tag{3.45}$$ eq:Gm3d

In the $d = 2, 3$ cases, the Green's function thus diverges at short distance, but in all cases $d = 1, 2, 3$ it decays exponentially at large distances, with characteristic correlation length $\xi = 1/m$.

Derivation: Answers: Explicit calculations for the free propagators

a) 1d: By simple contour integration,

$$\mathcal{G}_m(r) = \int \frac{dk}{2\pi} \frac{e^{-ikr}}{(k+im)(k-im)} = \frac{e^{-m|r|}}{2m}.$$

b) 2d:

$$\begin{aligned}\mathcal{G}_m(\boldsymbol{r})|_{d=2} = \int \frac{d^2k}{(2\pi)^2} \frac{e^{-i\mathbf{k}\cdot\boldsymbol{r}}}{k^2+m^2} &= \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_0^\infty dk k \frac{e^{-ik|\boldsymbol{r}|\cos\theta}}{k^2+m^2} \\ &= \frac{1}{2\pi^2} \int_0^\infty dk \frac{k}{k^2+m^2} \int_0^\pi d\theta \cos(k|\boldsymbol{r}|\cos\theta)\end{aligned}$$

We can now use the identity (c.f. Gradshteyn & Ryzhik 3.715.18)

$$\int_0^\pi d\theta \cos(z\cos\theta)\cos n\theta = \pi \cos\frac{n\pi}{2} J_n(z)$$

where J_n is the n-th Bessel function of the first kind. Substituting, we get

$$\mathcal{G}_m(\boldsymbol{r})|_{d=2} = \frac{1}{2\pi} \int_0^\infty dk \frac{kJ_0(k|\boldsymbol{r}|)}{k^2+m^2} = \frac{1}{2\pi} K_0(m|\boldsymbol{r}|)$$

in which we have used GR 6.532.4,

$$\int_0^\infty dk \frac{kJ_0(kr)}{k^2+m^2} = K_0(mr)$$

in which K_n is the modified Bessel function of the second kind (here with $n = 0$).

The limits for small and large values of $|\boldsymbol{r}|$ can be obtained from the asymptotic forms of Bessel functions at small argument,

$$\begin{aligned} K_0(z) &= -\ln\frac{z}{2}I_0(z) + \sum_{k=0}^{\infty} z^{2k}2^{2k}(k!)^2\psi(k+1) \quad \text{GR 8.447.3,} \\ I_0(z) &= \sum_{k=0}^{\infty}\frac{(z/2)^{2k}}{(k!)^2} \quad \text{GR 8.447.1,} \end{aligned}$$

or at large argument

$$K_\nu(z) = \sqrt{\frac{\pi}{2z}}e^{-z}\,[1+...] \quad \text{GR 8.454.6.}$$

c) 3d:

$$\mathcal{G}_m(\boldsymbol{r})|_{d=3} = \frac{1}{(2\pi)^3}\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\sin\theta\int_0^{\infty}dkk^2\frac{e^{-ik|\boldsymbol{r}|\cos\theta}}{k^2+m^2}.$$

Let $z = \cos\theta$. We get

$$\mathcal{G}_m(\boldsymbol{r})|_{d=3} = \frac{1}{4\pi^2}\int_0^{\infty}dk\frac{k^2}{k^2+m^2}\int_{-1}^{1}dze^{-ik|\boldsymbol{r}|z} = \frac{1}{2\pi^2|\boldsymbol{r}|}\int_0^{\infty}dk\frac{k\sin(k|\boldsymbol{r}|)}{k^2+m^2}$$

This integral is tabulated,

$$\int_{-\infty}^{\infty}dx\frac{x\sin(ax)}{x^2+b^2} = \pi e^{-ab} \qquad a>0, \Re b>0 \qquad \text{GR 3.723.4}$$

which gives the final result.

3.1.3 The path integral

It is straightforward to express the properties of the motion of our random walker in terms of sums over the paths which can be taken. We can immediately write

$$P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = \frac{\text{Number of paths joining } \boldsymbol{r}_0 \text{ to } \boldsymbol{r}_1 \text{ with } \frac{t_1-t_0}{\delta t} \text{ steps}}{\text{Total number of paths out of } \boldsymbol{r}_0 \text{ with } \frac{t_1-t_0}{\delta t} \text{ steps}}. \tag{3.46}$$

Let us work directly in the scaling limit. From (3.21), we have that for initial and final positions and times $\boldsymbol{r}_i, t_i$ and $\boldsymbol{r}_f, t_f$, the probability density of finding the particle was given by the exact (in the scaling limit) expression

$$p(\boldsymbol{r}_f,t_f|\boldsymbol{r}_i,t_i) = \frac{1}{[4\pi D(t_f-t_i)]^{\frac{d}{2}}}\exp\left[-\frac{|\boldsymbol{r}_f-\boldsymbol{r}_i|^2}{4D(t_f-t_i)}\right]. \tag{3.47}$$

On the other hand, we have the composition property (3.26) which can be concatenated. Let us imagine that we split our time interval $t_f - t_i$ into N equal intervals of duration $\frac{t_f-t_i}{N} \equiv \Delta t$ (identifying $\boldsymbol{r}_0 \equiv \boldsymbol{r}_i, t_0 \equiv t_i$ and $\boldsymbol{r}_N \equiv \boldsymbol{r}_f, t_N \equiv t_f$), and apply (3.26) at each $N-1$ intermediate time step:

$$p(\boldsymbol{r}_f,t_f|\boldsymbol{r}_i,t_i) = \int\prod_{n=1}^{N-1}d^d\boldsymbol{r}_n p(\boldsymbol{r}_f,t_f|\boldsymbol{r}_{N-1},t_{N-1})p(\boldsymbol{r}_{N-1},t_{N-1}|\boldsymbol{r}_{N-2},t_{N-2})...p(\boldsymbol{r}_1,t_1|\boldsymbol{r}_i,t_i). \tag{3.48}$$

In the limit $N \to \infty$, the time steps Δt become infinitesimal (remember that we are working directly in the scaling limit: at each time step here, there are still infinitely many steps being

taken on the original lattice, in other words we still have $\delta t/\Delta t = 0$). For an infinitesimal time step, we can write

$$p(\boldsymbol{r}_{n+1}, t_{n+1}|\boldsymbol{r}_n, t_n) \underset{t_{n+1}-t_n=\Delta t\to 0^+}{\longrightarrow} \frac{1}{[4\pi D\Delta t]^{\frac{d}{2}}} \exp\left[-\frac{\Delta t}{4D}\left|\frac{\Delta \boldsymbol{r}(t_n)}{\Delta t}\right|^2\right] \tag{3.49}$$

where

$$\frac{\Delta \boldsymbol{r}(t_n)}{\Delta t} \equiv \frac{\boldsymbol{r}_{n+1}-\boldsymbol{r}_n}{\Delta t} \to \frac{d\boldsymbol{r}(t)}{dt}. \tag{3.50}$$

We can thus write our probability as the **path integral**

$$p(\boldsymbol{r}_f, t_f|\boldsymbol{r}_i, t_i) = \int\limits_{\substack{\boldsymbol{r}(t_i)=\boldsymbol{r}_i\\ \boldsymbol{r}(t_f)=\boldsymbol{r}_f}} \mathcal{D}\boldsymbol{r}(t) \exp\left[-\frac{1}{4D}\int_{t_i}^{t_f} dt \left|\frac{d\boldsymbol{r}(t)}{dt}\right|^2\right] \tag{3.51}$$

where the **path integral measure** is here defined as

$$\int\limits_{\substack{\boldsymbol{r}(t_i)=\boldsymbol{r}_i\\ \boldsymbol{r}(t_f)=\boldsymbol{r}_f}} \mathcal{D}\boldsymbol{r}(t) F[\boldsymbol{r}(t)] \equiv \lim_{N\to\infty}\left[\frac{N}{4\pi D(t_f-t_i)}\right]^{Nd/2} \int \prod_{n=1}^{N-1} d\boldsymbol{r}_n F(\{\boldsymbol{r}_n\})\Big|_{\substack{\boldsymbol{r}_0=\boldsymbol{r}_i\\ \boldsymbol{r}_N=\boldsymbol{r}_f}} \tag{3.52}$$

where $F[\boldsymbol{r}(t)]$ is the functional corresponding to the function $F(\{\boldsymbol{r}_n\})$.

For the exhaustible walker, we simply use (3.32) and the limits (recalling (3.14))

$$\lim(1-\eta)^{\frac{t_f-t_i}{\delta t}} = \lim\left(1-\frac{a^2}{2d}m^2\right)^{\frac{t_f-t_i}{\delta t}} = e^{-(t_f-t_i)Dm^2} \tag{3.53}$$

so we simply have

$$p_m(\boldsymbol{r}_f, t_f|\boldsymbol{r}_i, t_i) = e^{-(t_f-t_i)Dm^2} p(\boldsymbol{r}_f, t_f|\boldsymbol{r}_i, t_i). \tag{3.54}$$

For the Green's function, we have

$$\mathcal{G}_m(\boldsymbol{r}) = \lim \frac{a^2}{2d}\sum_{n=0}^{\infty} p_m(\boldsymbol{r}, n\delta t|\boldsymbol{0}, 0) \tag{3.55}$$

and we therefore obtain the path integral representation

$$\mathcal{G}_m(\boldsymbol{r}) = D\int_0^\infty dt \int\limits_{\substack{\boldsymbol{r}(0)=\boldsymbol{0}\\ \boldsymbol{r}(t)=\boldsymbol{r}}} \mathcal{D}\boldsymbol{r}(t') \exp\left[-\int_0^t dt'\left(Dm^2 + \frac{1}{4D}\left|\dot{\boldsymbol{r}}(t')\right|^2\right)\right]. \tag{3.56}$$

eq:GPI

A few comments are in order. Why did we even bother to define such a path integral, given that we had the exact solution for any initial/final positions in equation (3.21)? The reason is of course that while we were able to provide such an exact solution for this particular case, this is by no means the usual situation. In most circumstances, we cannot solve the time evolution equations exactly, and must be content with some form of approximation. The time evolution is implemented by an evolution equation of the form (3.24) but generically containing other terms whose effects cannot be tracked exactly. One then relies on approximations (for example that the relevant dynamics is restricted to some low-energy/slow-changing configurations). Dividing the time evolution into microscopic time steps as we have done here is then still meaningful: expressions corresponding to (3.56) can always be written down irrespective of how our time evolution occurs, whereas solutions like (3.21) are more often than not too much to wish for.

3.1.4 Visit and return probabilities

Let us now return to the random walker on the hypercubic lattice (before taking the scaling limit), and address a slightly different question: what is the probability $\Pi_{\boldsymbol{r},t}$ that the walker has trodden at least once on site $\boldsymbol{r}$ by time t, given that it started at $\boldsymbol{r}_0 \equiv \boldsymbol{0}$ at time $t_0 \equiv 0$? For the special case $\boldsymbol{r} = \boldsymbol{r}_0$, this is known as the **return probability**[5].

The probabilities $P_{\boldsymbol{r},t}$[6] are not exactly what we are looking for (though it is intimately related): summing these over all times would give the mean time spent at site $\boldsymbol{r}$. Instead, let us define the intermediate quantities $P_{\boldsymbol{r},t;i}$ of being at site $\boldsymbol{r}$ for the i-th time at time t. We then have that

$$P_{\boldsymbol{r},t} = \delta_{\boldsymbol{r},\boldsymbol{0}}\delta_{t,0} + \sum_{i=1}^{\infty} P_{\boldsymbol{r},t;i}. \tag{3.57}$$

Note that only a finite number of terms contribute to this sum, since $P_{\boldsymbol{r},t;i} = 0$ for $i > t/\delta t$. Note also that our definitions are such that $P_{\boldsymbol{r},0;i} = 0$. Since an $i+1$-th visit necessarily follows an i-th visit, we can write the recurrence relation (using homogeneity of the walk in space and time)

$$P_{\boldsymbol{r},t;i+1} = \sum_{t_1+t_2=t} P_{\boldsymbol{r},t_1;i} P_{\boldsymbol{0},t_2;1}. \tag{3.58}$$

The summation of this relation over $i = 1, ..., \infty$ then yields

$$P_{\boldsymbol{r},t} - P_{\boldsymbol{r},t;1} - \delta_{\boldsymbol{r},\boldsymbol{0}}\delta_{t,0} = \sum_{t_1+t_2=t} P_{\boldsymbol{r},t_1} P_{\boldsymbol{0},t_2;1} - \delta_{\boldsymbol{r},\boldsymbol{0}} P_{\boldsymbol{r},t;1}. \tag{3.59}$$

The probability of having visited site $\boldsymbol{r}$ at least once is then

$$\Pi_{\boldsymbol{r}} = \sum_{t=0}^{\infty} P_{\boldsymbol{r},t;1}. \tag{3.60}$$

Treating the more general case of the exhaustible walker, we can simply replace all the P by $P^{(\eta)}$, giving for example

$$P^{(\eta)}_{\boldsymbol{r},t} - P^{(\eta)}_{\boldsymbol{r},t;1} - \delta_{\boldsymbol{r},\boldsymbol{0}}\delta_{t,0} = \sum_{t_1+t_2=t} P^{(\eta)}_{\boldsymbol{r},t_1} P^{(\eta)}_{\boldsymbol{0},t_2;1} - \delta_{\boldsymbol{r},\boldsymbol{0}} P^{(\eta)}_{\boldsymbol{r},t;1}. \tag{3.61}$$

Using

$$\Pi^{(\eta)}_{\boldsymbol{r}} = \sum_{t=0}^{\infty} P^{(\eta)}_{\boldsymbol{r},t;1}, \qquad \Pi_{\boldsymbol{r}} = \lim_{\eta\to 0} \Pi^{(\eta)}_{\boldsymbol{r}}, \tag{3.62}$$

and summing over time gives

$$\mathcal{G}^{(\eta)}_{\boldsymbol{r}} = \delta_{\boldsymbol{r},\boldsymbol{0}} + [1 - \delta_{\boldsymbol{r},\boldsymbol{0}}]\, \Pi^{(\eta)}_{\boldsymbol{r}} + \mathcal{G}^{(\eta)}_{\boldsymbol{r}} \Pi^{(\eta)}_{\boldsymbol{0}}. \tag{3.63}$$

This gives us two very aesthetic equations: first of all, the return probability is simply expressed in terms of the Green's function at zero distance:

$$\Pi^{(\eta)}_{\boldsymbol{0}} = 1 - \frac{1}{\mathcal{G}^{(\eta)}_{\boldsymbol{0}}}. \tag{3.64}$$

[5] In here and all further considerations, we assume that the walker has *left* the origin, so we exclude the initial state at the initial time.

[6] Dropping the $\boldsymbol{r}_0, t_0$ arguments for notational simiplicity. Remember that our random walk is homogeneous in space and (discrete) time.

Second, the visit probability at site $\boldsymbol{r}$ is simply given by the ratio of the Green's function at that point to that at the origin:

$$\Pi_{\boldsymbol{r}}^{(\eta)} = \frac{\mathcal{G}_{\boldsymbol{r}}^{(\eta)}}{\mathcal{G}_{\boldsymbol{0}}^{(\eta)}}, \qquad \boldsymbol{r} \neq \boldsymbol{0}. \tag{3.65}$$

Some comments are in order. We know that for $d \leq 2$, $\lim_{\eta \to 0} \mathcal{G}_{\boldsymbol{r}}^{(\eta)} \to \infty$ uniformly for any $\boldsymbol{r}$, so $\Pi_{\boldsymbol{0}} \to 1$ and $\Pi_{\boldsymbol{r}} \to 1$ for any $\boldsymbol{r}$. For $d > 2$ the return probability is less than one, and decreases as $1/d$ for large d.

3.2 The Feynman path integral in quantum mechanics

Let us now move to the realm of quantum mechanics. Instead of the time evolution being driven by a stochastic process as in the case of Brownian motion, our system will now obey the deterministic Schrödinger equation.

The path integral formulation of quantum mechanics was initiated by P.A.M. Dirac, but pushed to new heights by R. P. Feynman. The book by Feynman & Hibbs contains a detailed exposition of the method.

The path integral formulation of quantum mechanics possesses a number of advantages over the standard formulation.

1. the classical limit ($\hbar \to 0$) is clear
2. it provides road towards non-perturbative methods
3. it serves as a prototype for the functional field integral
4. it has many direct applications for systems with one degree of freedom.

Our starting point to formulate the path integral is to perform a formal integration of the time-dependent Schrödinger equation:

$$i\hbar\partial_t|\Psi\rangle = \hat{H}|\Psi\rangle \quad \to \quad |\Psi(t')\rangle = \hat{U}(t',t)|\Psi(t)\rangle, \qquad \hat{U}(t',t) = e^{-\frac{i}{\hbar}\hat{H}(t'-t)}. \tag{3.66}$$

Considering the simplest situation in which we have a single particle evolving in a continuum interval (with the position labeled by q), we can write the wavefunction in the real space representation as

$$\Psi(q',t') = \langle q'|\Psi(t')\rangle = \langle q'|\hat{U}(t',t)|\Psi(t)\rangle = \int dq\; U(q',t';q,t)\Psi(q,t) \tag{3.67}$$

where the time-evolution operator has matrix elements

$$U(q',t';q,t) = \langle q'|e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|q\rangle \tag{3.68}$$

Since this matrix element represents the probability amplitude for a particle to propagate from points q to point q' in a time $t'-t$, this is known as the **propagator** of the theory.

The basic idea behind Feynman's path integral is to split the finite time interval into infinitesimal chunks Δt, such that $t = N\Delta t$ with $N \gg 1$. The time evolution operator then factorizes into a product of time-step operators,

$$e^{-\frac{i}{\hbar}\hat{H}t} = \left[e^{-\frac{i}{\hbar}\hat{H}\Delta t}\right]^N. \tag{3.69}$$

CMFT(3.2)

Assuming that the Hamiltonian takes the form of the sum of a kinetic and a potential part, $\hat{H} = \hat{T} + \hat{V}$, we can factorize the time-step operator according to

$$e^{-\frac{i}{\hbar}\hat{H}\Delta t} = e^{-\frac{i}{\hbar}\hat{T}\Delta t}e^{-\frac{i}{\hbar}\hat{V}\Delta t} + O(\Delta t^2) \tag{3.70}$$

in which the $O(\Delta t^2)$ error is proportional to the commutator of $\hat{T}$ and $\hat{V}$. The truncation of this power-series expansion in Δt thus makes sense if Δt is much smaller than the reciprocal of the matrix elements of this commutator. Since our number N of time slices can be chosen to be arbitrarily large, the expansion formally converges.

The propagator can then be approximated by

$$\langle q_f|\left[e^{-\frac{i}{\hbar}\hat{H}\Delta t}\right]^N|q_i\rangle \simeq \langle q_f|\mathbf{1}_N e^{-\frac{i}{\hbar}\hat{T}\Delta t}e^{-\frac{i}{\hbar}\hat{V}\Delta t}\mathbf{1}_{N-1}...\mathbf{1}_1 e^{-\frac{i}{\hbar}\hat{T}\Delta t}e^{-\frac{i}{\hbar}\hat{V}\Delta t}|q_i\rangle \tag{3.71}$$

in which $\mathbf{1}$ are fixed time-slice resolutions of the identity operator, each being the product of resolutions of the identity in q and p space,

$$\begin{aligned}\mathbf{1}_n = \mathbf{1}_{q_n}\mathbf{1}_{p_n} = \int dq_n|q_n\rangle\langle q_n| \int dp_n|p_n\rangle\langle p_n| = \int dq_n dp_n|q_n\rangle\langle p_n|(\langle q_n|p_n\rangle) \\ = \int dq_n dp_n|q_n\rangle\langle p_n|\frac{e^{\frac{i}{\hbar}q_n p_n}}{\sqrt{2\pi\hbar}}\end{aligned} \tag{3.72}$$

in which we have used the convention $\langle p|q\rangle = \langle q|p\rangle^* = e^{-\frac{i}{\hbar}qp}/\sqrt{2\pi\hbar}$. Assuming that $\hat{T}$ is diagonalized by states $|p\rangle$, and $\hat{V}$ by states $|q\rangle$), we obtain

$$\begin{aligned}\langle q_f|e^{-\frac{i}{\hbar}\hat{H}t}|q_i\rangle \simeq \int \prod_{n=1}^{N}\frac{dq_n dp_n}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}q_n p_n}\langle q_f|q_N\rangle\langle p_N|e^{-\frac{i}{\hbar}T(p_N)\Delta t}e^{-i\frac{i}{\hbar}V(q_{N-1})\Delta t}|q_{N-1}\rangle \times \\ \times\langle p_{N-1}|e^{-\frac{i}{\hbar}T(p_{N-1})\Delta t}e^{-i\frac{i}{\hbar}V(q_{N-2})\Delta t}|q_{N-2}\rangle \times ... \times |q_i\rangle.\end{aligned} \tag{3.73}$$

The T and V exponentials are now simple numbers, and can be taken out of the bra-ket inner products. Substituting again the projection coefficients $\langle p_n|q_{n-1}\rangle = e^{-\frac{i}{\hbar}p_n q_{n-1}}/\sqrt{2\pi\hbar}$ in this equation, we get

$$\langle q_f|e^{-\frac{i}{\hbar}\hat{H}t}|q_i\rangle \simeq \int \prod_{n=1}^{N-1}dq_n \prod_{n=1}^{N}\frac{dp_n}{2\pi\hbar}e^{-i\frac{\Delta t}{\hbar}\sum_{n=0}^{N-1}(T(p_{n+1})+V(q_n)-p_{n+1}\frac{q_{n+1}-q_n}{\Delta t})}|_{q_N=q_F,q_0=q_i}. \tag{3.74}$$

This is exact up to corrections of order $[\hat{T},\hat{V}]\Delta t^2/\hbar^2$.

The remarkable thing about (3.74) is that the left-hand side, a quantum-mechanical transition amplitude, is expressed purely in terms of (an integration over) classical phase-space variables $x_n = (q_n, p_n)$. The constant $\hbar$, and the fact that we are summing a complex-valued integrand, are the only leftovers of the original Schrødinger time evolution equation.

Let us now briefly discuss the behaviour of the integral (3.74). The first thing to notice is that rapid fluctuations of the arguments x_n as a function of n are strongly inhibited (since the integrand is oscillatory). Contributions for which $(q_{n+1}-q_n)p_{n+1} > O(\hbar)$ tend to cancel each other because of destructive interference. The only contributions which survive are from paths which are smooth in space-time, which allows us to take the limit $N\to\infty$ (keeping $t = N\Delta t$ fixed) and rewrite the product of phase-space integrals in terms of a path integral: the set of points $\{x_n\}$ becomes a curve $x(t)$, and

$$\begin{aligned}\Delta t\sum_{n=0}^{N-1}\to\int_0^t dt', \qquad \frac{q_{n+1}-q_n}{\Delta t}\to\partial_{t'}q|_{t'=t_n}\equiv\dot{q}|_{t'=t_n}, \\ T(p_{n+1})+V(q_n)\to T(p|_{t'=t_n})+V(q|_{t'=t_n})\equiv H(x|_{t'=t_n})\end{aligned} \tag{3.75}$$

i.e. the *classical* Hamiltonian. Then,

$$\lim_{N\to\infty}\int\prod_{n=1}^{N-1}dq_n\prod_{n=1}^{N}\frac{dp_n}{2\pi\hbar}(...)|_{q_N=q_f,q_0=q_i}\equiv\int\mathcal{D}x(...)|_{q(t)=q_f,q(0)=q_i} \tag{3.76}$$

defines the path integral measure. Finally, one gets for the propagator

$$\langle q_f|e^{-\frac{i}{\hbar}\hat{H}t}|q_i\rangle = \int \mathcal{D}x \, \exp\left[\frac{i}{\hbar}\int_0^t dt'(p\dot{q} - H(p,q))\right]|_{q(t)=q_f,q(0)=q_i} \tag{3.77}$$ CMFT(3.6)

which is the **Hamiltonian formulation of the path integral**.

In the specific case of free dynamics, $\hat{T} = \frac{\hat{p}^2}{2m}$, we can explicitly perform the (functional) Gaussian integral over momentum and obtain

$$\langle q_f|e^{-\frac{i}{\hbar}\hat{H}t}|q_i\rangle = \int \mathcal{D}x \; e^{-\frac{i}{\hbar}\int_0^t dt' V(q)} \times e^{-\frac{i}{\hbar}\int_0^t dt'(\frac{p^2}{2m} - p\dot{q})}|_{q(t)=q_f,q(0)=q_i} \tag{3.78}$$ CMFT(3.7)

$$= \int \mathcal{D}q \, \exp\left[\frac{i}{\hbar}\int_0^t dt' L(q,\dot{q})\right]|_{q(t)=q_f,q(0)=q_i} = \int \mathcal{D}q \, \exp\left[\frac{i}{\hbar}S[q,\dot{q}]\right]|_{q(t)=q_f,q(0)=q_i} \tag{3.79}$$ CMFT(3.8)

with $L(q,\dot{q}) = \frac{m}{2}\dot{q}^2 - V(q)$ is the classical Lagrangian, $S[q,\dot{q}]$ is the action functional, and

$$\mathcal{D}q = \lim_{N\to\infty}\left(\frac{Nm}{it2\pi\hbar}\right)^{N/2}\prod_{n=1}^{N-1} dq_n \tag{3.80}$$

is the functional measure of the remaining integral.

Therefore: a *quantum mechanical* transition amplitude has been expressed in terms of a *path integral* through phase space or coordinate space, weighed by the classical action. This is Dirac's 'sum over histories' idea, pushed by Feynman.

Gaussian functional integration [supplement to PRELIMINARIES on Gaussian integration] Starting from (CMFT(3.13) A.19), suppose that the vector **v** parametrizes the weight of a real scalar field on the sites of a one-dimensional lattice. In continuum limit: set $\{v_i\}$ becomes a function $v(x)$ and the matrix A_{ij} becomes an **operator kernel** or **propagator** $A(x,x')$. Natural generalization of (CMFT(3.13) A.19):

$$\int \mathcal{D}v(x) \, \exp\left[-\frac{1}{2}\int dxdx' v(x)A(x,x')v(x') + \int dx j(x)v(x)\right]$$
$$= (\det\,\frac{A}{2\pi})^{-1/2}\,\exp\left[\frac{1}{2}\int dxdx' j(x)A^{-1}(x,x')j(x')\right] \tag{3.81}$$

where the inverse kernel satisfies

$$\int dx' A(x,x')A^{-1}(x',x'') = \delta(x-x'') \tag{3.82}$$ CMFT(3.20)

so $A^{-1}(x,x')$ is the **Green function** of the operator $A(x,x')$.

Equation (CMFT(3.14) A.20) generalizes to

$$\langle v(x)v(x')\rangle = A^{-1}(x,x') \tag{3.83}$$

and (CMFT(3.16) A.23) generalizes to

$$\langle v(x_1)v(x_2)...v(x_{2n})\rangle = \sum_{pairings} A^{-1}(x_{k_1},x_{k_2})...A^{-1}(x_{k_{2n-1}},x_{k_{2n}}). \tag{3.84}$$ CMFT(3.21)

The path integral for a free particle

For a free particle $\hat{H} = \frac{\hat{p}^2}{2m}$, $\hat{L} = \frac{m}{2}\hat{\dot{q}}^2$, we have

$$G_{\text{free}}(q_f, q_i; t) \equiv \langle q_f | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t} | q_i \rangle = \lim_{N\to\infty} \left(\frac{Nm}{it2\pi\hbar}\right)^{N/2} \int \prod_{n=1}^{N-1} dq_n e^{\frac{i}{\hbar}\int_0^t dt' \frac{m}{2}(\frac{dq}{dt'})^2}. \tag{3.85}$$

We choose $q_0 = q_i$ and $q_N = q_f$, with $t = N\Delta t$. The action can be written

$$\frac{m}{2}\int_0^t dt'(\frac{dq}{dt'})^2 = \frac{m}{2}\Delta t \sum_{n=1}^{N}(\frac{q_n - q_{n-1}}{\Delta t})^2 = \frac{m}{2\Delta t}\sum_{n=1}^{N}(q_n - q_{n-1})^2. \tag{3.86}$$

Look at the integral for q_1:

$$\begin{aligned}\int_{-\infty}^{\infty} dq_1 e^{\frac{im}{2\hbar\Delta t}((q_2-q_1)^2+(q_1-q_0)^2)} &= \int_{-\infty}^{\infty} dq_1 e^{\frac{im}{2\hbar\Delta t}(2q_1^2 - 2q_1(q_0+q_2)+q_2^2+q_0^2)} \\ = \int_{-\infty}^{\infty} dq_1 e^{\frac{im}{2\hbar\Delta t}*2((q_1-\frac{q_0+q_2}{2})^2-(\frac{q_0+q_2}{2})^2+\frac{q_2^2+q_0^2}{2})} &= I(-\frac{2im}{\hbar\Delta t})e^{\frac{im}{2\hbar\Delta t}\frac{(q_2-q_0)^2}{2}} \\ &= \left(\frac{2\pi i\hbar\Delta t}{2m}\right)^{1/2} e^{\frac{im}{2\hbar\Delta t}\frac{(q_2-q_0)^2}{2}}\end{aligned} \tag{3.87}$$

Now look at the integral for q_2:

$$\begin{aligned}\int_{-\infty}^{\infty} dq_2 e^{\frac{im}{2\hbar\Delta t}((q_3-q_2)^2+\frac{1}{2}(q_2-q_0)^2)} &= \int_{-\infty}^{\infty} dq_2 e^{\frac{im}{2\hbar\Delta t}(\frac{3}{2}q_2^2 - q_2(2q_3+q_0)+q_3^2+\frac{q_0^2}{2})} \\ &= \int_{-\infty}^{\infty} dq_2 e^{\frac{im}{2\hbar\Delta t}(\frac{3}{2}(q_2-\frac{2q_3+q_0}{3})^2-\frac{3}{2}(\frac{2q_3+q_0}{3})^2+q_3^2+\frac{q_0^2}{2})} \\ &= \left(\frac{2\pi\hbar i\Delta t}{m} * \frac{2}{3}\right)^{1/2} e^{\frac{im}{2\hbar\Delta t}(-\frac{2}{3}(q_3+q_0/2)^2+q_3^2+\frac{q_0^2}{2})}.\end{aligned} \tag{3.88}$$

But we have $-\frac{2}{3}(q_3+q_0/2)^2 + q_3^2 + \frac{q_0^2}{2} = \frac{(q_3-q_0)^2}{3}$ so after the q_2 integral, we have

$$\left(\frac{2\pi\hbar i\Delta t}{m} * \frac{1}{2}\right)^{1/2}\left(\frac{2\pi\hbar i\Delta t}{m} * \frac{2}{3}\right)^{1/2} e^{\frac{im}{2\hbar\Delta t}\frac{(q_3-q_0)^2}{3}}. \tag{3.89}$$

Carrying on with the $q_3, ..., q_{N-1}$ integrals then gives

$$\left(\frac{2\pi\hbar i\Delta t}{m}\right)^{\frac{N-1}{2}} * \left(\frac{1}{N}\right)^{1/2} e^{\frac{im}{2\hbar\Delta t}\frac{(q_N-q_0)^2}{N}}. \tag{3.90}$$

By using $t = N\Delta t$ and $q_f = q_N, q_i = q_0$, we thus finally get

$$G_{\text{free}}(q_f, q_i; t) = \left(\frac{m}{2\pi\hbar it}\right)^{1/2} e^{\frac{im}{2\hbar t}(q_f-q_i)^2}. \tag{3.91}$$

CMFT(3.29)

The path integral for a free particle: alternative derivation using matrix Gaussian integration

The action can be written using

$$\sum_{n=1}^{N}(q_n - q_{n-1})^2 = q_0^2 + q_N^2 + \boldsymbol{q}^T \boldsymbol{M}_{N-1}\boldsymbol{q} - 2\boldsymbol{J}^T \cdot \boldsymbol{q} \tag{3.92}$$

where we have defined the $N-1$-dimensional vectors

$$\boldsymbol{q}^T \equiv \begin{pmatrix} q_1 & ... & q_{N-1} \end{pmatrix}, \qquad \boldsymbol{J}^T \equiv \begin{pmatrix} q_0 & 0 & ... & 0 & q_N \end{pmatrix}, \tag{3.93}$$

and the matrix (the supindex giving its dimension)

$$\boldsymbol{M}^{(\text{N-1})} = \begin{pmatrix} 2 & -1 & 0 & ... & 0 \\ -1 & 2 & -1 & 0 & ... \\ 0 & -1 & 2 & -1 & ... \\ ... & 0 & -1 & ... & -1 \\ 0 & ... & ... & -1 & 2 \end{pmatrix}. \tag{3.94}$$

We can calculate the determinant of $\boldsymbol{M}$ easily by for example putting all elements below the diagonal to zero, adding 1/2 times row 1 to row 2, etc.:

$$\text{Det}\boldsymbol{M} = \text{Det}\begin{pmatrix} 2 & -1 & 0 & ... & ... \\ 0 & 2-\frac{1}{2} & -1 & 0 & ... \\ 0 & -1 & 2 & -1 & ... \end{pmatrix} = \text{Det}\begin{pmatrix} d_1 & -1 & 0 & ... \\ 0 & d_2 & -1 & ... \\ 0 & 0 & d_3 & ... \end{pmatrix} \tag{3.95}$$

where

$$d_1 \equiv 2, \qquad d_{n+1} = 2 - \frac{1}{d_n} \qquad \Rightarrow \qquad d_n = \frac{n+1}{n}, \tag{3.96}$$

and thus

$$\text{Det}\boldsymbol{M}_{N-1} = N. \tag{3.97}$$

The free propagator can be written as

$$G_{\text{free}}(q_f, q_i; t) = \lim_{N\to\infty}\left(\frac{Nm}{it2\pi\hbar}\right)^{N/2} e^{\frac{im}{2\hbar\Delta t}(q_0^2+q_N^2)} \int \left[\prod_{n=1}^{N-1} dq_n\right] e^{-\frac{1}{2}\boldsymbol{q}^T\boldsymbol{A}\boldsymbol{q} + \boldsymbol{j}^T\cdot\boldsymbol{q}} \tag{3.98}$$

where

$$\boldsymbol{A} \equiv \frac{m}{i\hbar\Delta t}\boldsymbol{M}, \qquad \boldsymbol{j} \equiv \frac{m}{i\hbar\Delta t}\boldsymbol{J}. \tag{3.99}$$

The multivariable Gaussian integration can be performed using rule (CMFT(3.13) A.19), yielding

$$(2\pi)^{\frac{N-1}{2}}\ \text{Det}\ \mathbf{A}^{-1/2} e^{\frac{1}{2}\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}}. \tag{3.100}$$

In view of the structure of $\boldsymbol{J}$, the only inverse matrix elements we need are

$$\begin{aligned} (\boldsymbol{M}^{(\text{N-1})})^{-1}_{1,1} &= (\boldsymbol{M}^{(\text{N-1})})^{-1}_{N-1,N-1} = \frac{\text{Det}\boldsymbol{M}^{(\text{N-2})}}{\text{Det}\boldsymbol{M}^{(\text{N-1})}} = \frac{N-1}{N}, \\ (\boldsymbol{M}^{(\text{N-1})})^{-1}_{1,N-1} &= (\boldsymbol{M}^{(\text{N-1})})^{-1}_{N-1,1} = \frac{1}{\text{Det}\boldsymbol{M}^{(\text{N-1})}} = \frac{1}{N}, \end{aligned} \tag{3.101}$$

and thus

$$\boldsymbol{J}^T \boldsymbol{M}^{-1} \boldsymbol{J} = \frac{N-1}{N}(q_0^2 + q_N)^2 + \frac{2}{N} q_0 q_N = q_0^2 + q_N^2 - \frac{1}{N}(q_N - q_0)^2. \tag{3.102}$$

Collecting all factors then gives back the previous answer,

$$G_{\text{free}}(q_f, q_i; t) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{\frac{im}{2\hbar t}(q_f - q_i)^2}. \tag{3.103}$$

3.2.1 Correspondence between classical and quantum propagators

There is one striking aspect which can be noticed upon careful comparison of the quantum free particle probability amplitude for propagation (3.91),

$$G_{\rm free}(q_f,q_i;t)=\left(\frac{m}{2\pi\hbar it}\right)^{1/2}e^{\frac{im}{2\hbar t}(q_f-q_i)^2} \tag{3.104}$$

with the classical one (3.21) (specialized to one dimension), using τ to denote the 'classical' time interval

$$p(r_f,\tau|r_i,0)=\frac{1}{\left[4\pi D\tau\right]^{1/2}}\exp\left[-\frac{(r_f-r_i)^2}{4D\tau}\right]. \tag{3.105}$$

Explicitly, these expressions coincide under the identification

$$\tau=it\times\left(\frac{\hbar}{2Dm}\right). \tag{3.106}$$

The factor in parentheses is simply a scale for our clocks. More importantly, what should be noticed here is that there is a correspondence between quantum propagation in real(respectively: imaginary) time and classical propagation in imaginary(respectively: real) time. This could have been anticipated immediately from the starting point, by comparing the diffusion equation (3.24)

$$\frac{\partial}{\partial\tau}p(r_f,\tau|r_i,0)=D\nabla_f^2p(r_f,\tau|r_i,0)$$

with the Schrödinger equation for the free particle,

$$i\hbar\frac{\partial}{\partial t}U(q_f,t;q_i,0)=\frac{-\hbar^2}{2m}\nabla_f^2U(q_f,t;q_i,0).$$

This correspondence will also manifest itself at the level of general field theory, which will be treated in the following chapters. The mnemonic trick is that when going from classical to quantum, one should take $\tau\to it$.

3.2.2 An integral approximation method

One of the great aspects of the path integral formulation of a problem is that it is readily adaptable to approximation schemes.

To illustrate the idea, we begin with a very simple case. Consider a function $f(x)$ and the integral

$$I[f] = \int_{-\infty}^{\infty} dx e^{-f(x)}. \tag{3.107}$$

Knowing some features of the function f, what can we say about the functional $I[f]$? Suppose that $f(x)$ has a global minimum at x_0. The integrand will be largest in the region where f has this minimum. Expanding f, we get

$$I[f] = \int_{-\infty}^{\infty} dx e^{-f(x_0)-\frac{a}{2}(x-x_0)^2+\mathcal{O}((x-x_0)^3)} = e^{-f(x_0)} G_a(1+...) \tag{3.108}$$

in which $a \equiv \frac{d^2}{dx^2} f|_{x_0}$ (since x_0 represents a minimum, we assume $a > 0$), $G_a \equiv \int_{-\infty}^{\infty} dx e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}$ is the Gaussian integral and ... represent corrections (which can be systematically computed in terms of fundamental integrals of the form $G_{a,n} \equiv \int_{-\infty}^{\infty} dx x^n e^{-\frac{a}{2}x^2}$). Note that the integral limits can be adapted here: to a certain degree of accuracy, provided the minimum point x_0 sits in the bulk of the original integration interval and that $f(x)$ becomes sufficiently large away from x_0, the boundaries can be put to $\pm\infty$. Note that the steeper the minimum of $f(x)$ is, the more accurate the approximation is. Note also that if f has multiple minima, then one can simply sum over the Gaussian-like integrals over each of these minima to approximate the full integral.

As an example, we can consider the integral representation of the Gamma function

$$\Gamma(z+1) = \int_0^{\infty} dx x^z e^{-x}. \tag{3.109}$$

Following our procedure gives

$$\begin{aligned} &\Gamma(z+1) = \int_0^{\infty} dx e^{-x+z\ln x}, \qquad f(x) = x - z\ln x, \qquad x_0 = z, \qquad f(x_0) = z(1-\ln z), \\ &a = d_x^2 f(x)|_{x_0} = z/x^2|_{x_0} = 1/z, \qquad \sqrt{2\pi/a} = \sqrt{2\pi z}. \end{aligned} \tag{3.110}$$

We thus directly obtain Stirling's approximation,

$$\Gamma(z+1) = \sqrt{2\pi z} e^{z(\ln z - 1)}(1+...). \tag{3.111}$$

This approximation method is also valid when dealing with a complex-valued argument in the integrand's exponential. It is generally known as the **stationary phase approximation**.

3.2.3 Stationary phase approximation of path integrals

Let us now adapt this idea to path integrals. Consider the functional integral $\int \mathcal{D}x e^{-F[x]}$ where $\mathcal{D}x = \lim_{N\to\infty} \prod_{n=1}^{N} dx_n$. As before, we are integrating over a set of fixed time-slice coordinates becoming a smooth function of time in the limit $N \to \infty$, $\{x_n\} \to x(t)$ with t playing the role of the former index n. The functional $F[x]$ depends on $x(t)$ at any t.

Evaluating this functional integral in the stationary phase approximation consists is performing the following steps:

1. Find the points of stationary phase, *i.e.* configurations $\bar{x}(t)$ such that the functional derivative of the action vanishes,

$$D_x F = 0 \Leftrightarrow \frac{\delta F[x]}{\delta x(t)} = 0 \ \forall t. \tag{3.112}$$

2. Perform a (functional) Taylor expansion of F to second order around $\bar{x}$:

$$F[x] = F[\bar{x}+y] = F[\bar{x}] + \frac{1}{2}\int dt dt' y(t') A(t,t') y(t) + ... \tag{3.113}$$ CMFT(3.24)

where $A(t,t') = \frac{\delta^2 F[x]}{\delta x(t)\delta x(t')}|_{x=\bar{x}}$. The first-order term is zero because of the stationarity condition.

3. Check that kernel $\hat{A} \equiv \{A(t,t')\}$ is positive definite (thereby guaranteeing the convergence of the Gaussian approximation to the functional integral). If so, perform the functional integral over y, yielding $\int \mathcal{D}x e^{-F[x]} \simeq e^{-F[\bar{x}]} \det\left(\frac{\hat{A}}{2\pi}\right)^{-1/2}$ (see eq. (3.81)). CMFT(3.19)

4. Finally, if there are many stationary phase configurations $\bar{x}_i(t)$, simply sum over the individual contributions:

$$\int \mathcal{D}x e^{-F[x]} \simeq \sum_i e^{-F[\bar{x}_i]} \det\left(\frac{\hat{A}_i}{2\pi}\right)^{-1/2}. \tag{3.114}$$ CMFT(3.25)

To summarize, the stationary phase approximation is based on finding the dominant terms contributing to the functional integral, including the maximal points and their Gaussian approximation.

Let us now apply the stationary phase approximation to the Lagrangian form of the Feynman path integral for a single particle. In particular, this converges quickly in the semiclassical limit when we take $\hbar \to 0$. The dominant trajectory is the solution to the classical equations of motion, $\bar{q}(t) = q_{cl}(t)$. Defining deviations as $r(t) = q(t) - q_{cl}(t)$ (assuming that there is only one classical path) then leads to

$$\langle q_f | e^{-\frac{i}{\hbar}\hat{H}t} | q_i \rangle \simeq e^{\frac{i}{\hbar}S[q_{cl}]} \int_{r(0)=r(t)=0} \mathcal{D}r \exp\left[\frac{i}{2\hbar}\int_0^t dt' dt'' r(t') \frac{\delta^2 S[q]}{\delta q(t')\delta q(t'')}|_{q=q_{cl}} r(t'')\right] \tag{3.115}$$ CMFT(3.26)

which is the Gaussian approximation to the path integral.

For free Lagrangians $L(q,\dot{q}) = \frac{m}{2}\dot{q}^2 - V(q)$, the second functional derivative integral term is

computed most easily by Taylor expanding the action:

$$\begin{aligned} S[q] &= \int dt L(q,\dot{q}) = \int dt \left(\frac{m}{2}\dot{q}^2 - V(q)\right) \\ &= \int dt \left(\frac{m}{2}(\dot{q}_{cl}^2 + 2\dot{q}_{cl}\dot{r} + \dot{r}^2) - V(q_{cl}) - V'(q_{cl})r - \frac{1}{2}V''(q_{cl})r^2\right) + ... \\ &= S[q_{cl}] + \int dt \left(-m\ddot{q}_{cl}r - V'(q_{cl})r - \frac{m}{2}\ddot{r}r - \frac{1}{2}V''(q_{cl})r^2\right) + ... \\ &= S[q_{cl}] - \frac{1}{2}\int dt\ r(t)[m\partial_t^2 + V''(q_{cl}(t))]r(t) + ... \end{aligned} \tag{3.116}$$

with $V''(q_{cl}(t)) \equiv \partial_q^2 V(q)|_{q_{cl}(t)}$, so

$$\frac{1}{2}\int_0^t dt'dt'' r(t')\frac{\delta^2 S[q]}{\delta q(t')\delta q(t'')}|_{q=q_{cl}} r(t'') = -\frac{1}{2}\int_0^t dt' r(t')[m\partial_{t'}^2 + V''(q_{cl}(t'))]r(t'). \tag{3.117}$$

CMFT(3.27)

Doing the Gaussian integration finally yields the approximation

$$\begin{aligned} \langle q_f|e^{-\frac{i}{\hbar}\hat{H}t}|q_i\rangle \simeq e^{\frac{i}{\hbar}S[q_{cl}]} \int_{r(0)=r(t)=0} \mathcal{D}r\ \exp\left[-\frac{i}{2\hbar}\int dt' r(t')[m\partial_{t'}^2 + V''(q_{cl}(t'))]r(t')\right] \\ = e^{\frac{i}{\hbar}S[q_{cl}]}\ \det\left(\frac{i}{2\pi\hbar}[m\partial_t^2 + V''(q_{cl}(t))]\right)^{-1/2}. \end{aligned} \tag{3.118}$$

The path integral for the harmonic oscillator

Let us consider a particle in a harmonic potential, whose Hamiltonian and Lagrangian are respectively

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2, \qquad \hat{L} = \frac{m}{2}\dot{x}^2 - \frac{m\omega^2}{2}\hat{x}^2. \tag{3.119}$$

The propagator is then

$$G_{ho}(q_f, q_i; t) = \langle q_f | e^{-\frac{i}{\hbar}\hat{H}t} | q_i \rangle = \int \mathcal{D}q \; e^{\frac{i}{\hbar}S_{ho}[q]}\Big|_{q(t)=q_f, q(0)=q_i} \tag{3.120}$$

where

$$S_{ho}[q] = \int_0^t dt' L(q, \dot{q}) = \frac{m}{2}\int_0^t dt' \left(\dot{q}^2 - \omega^2 q^2\right). \tag{3.121}$$

The classical path is determined as

$$q_{cl}(t') = q_i \cos\omega t' + \left(\frac{q_f}{\sin\omega t} - q_i \cot\omega t\right)\sin\omega t' \tag{3.122}$$

so the classical action takes the value

$$S_{ho}[q_{cl}] = \frac{m\omega}{2\sin\omega t}\left((q_f^2 + q_i^2)\cos\omega t - 2q_f q_i\right). \tag{3.123}$$

The path integral itself can be calculated most easily using our expression (3.118), which is exact since our Hamiltonian is quadratic ($V'' = m\omega^2$). The deviations from the classical path can be expanded in Fourier modes

$$r(t') = \sum_{n=1}^{\infty} r_n \sin\frac{n\pi t'}{t}, \tag{3.124}$$

so we have

$$\int dt' r(t')\left[m\partial_{t'}^2 + V''\right] r(t') = \frac{mt}{2}\sum_{n=1}^{\infty} r_n^2 \left[\omega^2 - \frac{n^2\pi^2}{t^2}\right]. \tag{3.125}$$

The path integral over $r(t')$ then corresponds over a product of integrals over the r_n. To avoid dealing with the details of this transformation (Jacobian, etc), the easiest is to consider the ratio with the free propagator (so with $\omega = 0$) which we have already calculated:

$$\frac{\prod_n \int dr_n e^{-\frac{imt}{4\hbar}\left[\omega^2 - \frac{n^2}{\pi^2}t^2\right]r_n^2}}{\prod_n \int dr_n e^{-\frac{imt}{4\hbar}\left[-\frac{n^2}{\pi^2}t^2\right]r_n^2}} = \prod_{n=1}^{\infty}\left[1 - \frac{\omega^2 t^2}{n^2\pi^2}\right]^{-1/2} = \left[\frac{\sin\omega t}{\omega t}\right]^{-1/2}. \tag{3.126}$$

Using the explicit expression for our free propagator, we thus obtain the exact propagator for the quantum harmonic oscillator:

$$G_{ho}(q_f, q_i; t) = \left(\frac{m\omega}{2\pi i\hbar\sin\omega t}\right)^{1/2} e^{\frac{im\omega}{2\hbar\sin\omega t}\left((q_f^2 + q_i^2)\cos\omega t - 2q_i q_f\right)}. \tag{3.127}$$

Chapter 4

Functional integrals

FI

4. The functional field integral

4.1 Construction of the many-body path integral

Let us now generalized the previous chapter's single-particle ideas to the many-body case. The basic idea remains the same, namely to separate the (imaginary) time evolution into infinitesimal time slices, and absorb as much of dynamical phase in a set of suitable eigenstates.

For the many-body case, we shall need a more convenient basis of our Fock space. An appropriate basis would be one in which our creation/annihilation operators are somehow diagonal. We thus need eigenstates of these operators (whether this is even possible will be disscussed below). Such a basis is formed in practice using so-called **coherent states**.

4.1.1 Coherent states for bosons

Let us try to find eigenstates of the (bosonic) Fock space creation/annihilation operators $a, a^\dagger$.

N.B.: for fermions, anti-commutation of operators leads to anti-commutation of eigenvalues... we shall get back to this problem later.

Any state in Fock space, including the desired eigenstates $|\phi\rangle$ of bosonic Fock space operators $a, a^\dagger$, can be represented as a linear combination of our occupation number states:

$$|\phi\rangle = \sum_{n_1,n_2,\ldots} C_{n_1,n_2,\ldots}|n_1,n_2,\ldots\rangle, \qquad |n_1,n_2,\ldots\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}}\frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2!}}\ldots|0\rangle \tag{4.1}$$

with $|0\rangle$ the vacuum state.

An extremely important point to emphasize is that it is perfectly sensible to have a generic state $|\phi\rangle$ contain a superposition of basis states with different numbers of particles. This is in fact crucial if we are to find an eigenstate of our creation/annihilation operators. Namely, if the minimal number of particles in $|\phi\rangle$ is n_0, then the minimum number of particles in $a_i^\dagger|\phi\rangle$ is n_0+1. Therefore, if our vacuum is well-defined and there is no upper limit to the number of bosons we can introduce to the system, the creation operator $a^\dagger$ cannot have an eigenstate.

However, under those circumstances, annihilation operators a_i do possess eigenstates. These are known as **bosonic coherent states**, and are of the form

$$|\phi\rangle \equiv \exp\left[\sum_i \phi_i a_i^\dagger\right]|0\rangle \tag{4.2}$$ CMFT(4.1)

with $\phi = \{\phi_i\}$ a complex vector (i as usual labelling our single-particle states). That this state diagonalizes the annihilation operators can be verified explicitly:

$$\begin{aligned} a_i|\phi\rangle = a_i \exp\left[\sum_j \phi_j a_j^\dagger\right]|0\rangle &= \exp\left[\sum_{j\neq i} \phi_j a_j^\dagger\right] a_i e^{\phi_i a_i^\dagger}|0\rangle \\ = \exp\,[...]\sum_{n=0}^{\infty}\frac{\phi_i^n}{n!}a_i(a_i^\dagger)^n|0\rangle &= \exp\,[...]\sum_{n=1}^{\infty}\frac{\phi_i^n}{n!}n(a_i^\dagger)^{n-1}|0\rangle \\ = \exp\,[...]\,\phi_i\sum_{n=0}^{\infty}\frac{\phi_i^n}{n!}(a_i^\dagger)^n|0\rangle &= \phi_i|\phi\rangle. \end{aligned} \tag{4.3}$$

We thus indeed have

$$a_i|\phi\rangle = \phi_i|\phi\rangle, \qquad \forall i \tag{4.4}$$ CMFT(4.2)

so these coherent states in fact simultaneously diagonalize all annihilation operators. By taking the Hermitian conjugate of this relation, we get

$$\langle\phi| = \langle 0|\exp\sum_i \bar{\phi}_i a_i, \qquad \langle\phi|a_i^\dagger = \langle\phi|\bar{\phi}_i. \tag{4.5}$$ CMFT(4.3)

so our (dual) coherent states also diagonalize the creation operators $a_i^\dagger$ from the left (they are left-eigenstates of $a_i^\dagger$). Here, $\bar{\phi}_i = \phi_i^*$.

Although our creation operators $a_i^\dagger$ are not diagonalized by our coherent states, we can still compute their action on such a state:

$$\begin{aligned} a_i^\dagger|\phi\rangle = a_i^\dagger \exp\left[\sum_j \phi_j a_j^\dagger\right]|0\rangle &= \exp\left[\sum_{j\neq i} \phi_j a_j^\dagger\right] a_i^\dagger e^{\phi_i a_i^\dagger}|0\rangle \\ = \exp\left[\sum_{j\neq i}\phi_j a_j^\dagger\right]\partial_{\phi_i}e^{\phi_i a_i^\dagger}|0\rangle &= \partial_{\phi_i}|\phi\rangle. \end{aligned} \tag{4.6}$$

This is almost an eigenvalue equation; instead of replacing the quantum operator by a scalar value, we have simply replaced it by a differential operator on a scalar value. The crucial this is that the 'quantumness' of the operator has disappeared.

One can easily check that equations (4.4) and (4.6) are consistent with the canonical commutation relations: CMFT(4.2) CMFT(4.4)

$$\begin{aligned} [a_i, a_j^\dagger]|\phi\rangle &= a_i a_j^\dagger|\phi\rangle - a_j^\dagger a_i|\phi\rangle = a_i\partial_{\phi_j}|\phi\rangle - a_j^\dagger\phi_i|\phi\rangle \\ &= \partial_{\phi_j}a_i|\phi\rangle - \phi_i a_j^\dagger|\phi\rangle = \partial_{\phi_j}\phi_i|\phi\rangle - \phi_i\partial_j|\phi\rangle = \delta_{ij}|\phi\rangle. \end{aligned} \tag{4.7}$$

The overlap between two coherent states is given by a short explicit calculation as

$$\langle\theta|\phi\rangle = \langle 0|e^{\sum_i \bar{\theta}_i a_i}|\phi\rangle = e^{\sum_i \bar{\theta}_i\phi_i}\langle 0|\phi\rangle = e^{\sum_i \bar{\theta}_i\phi_i}\langle 0|0\rangle = e^{\sum_i \bar{\theta}_i\phi_i} \tag{4.8}$$

so

$$\langle\theta|\phi\rangle = \exp\left[\sum_i \bar{\theta}_i\phi_i\right]. \tag{4.9}$$ CMFT(4.5)

The norm of a coherent state is thus

$$\langle\phi|\phi\rangle = \exp\left[\sum_i \bar{\phi}_i\phi_i\right] \tag{4.10}$$ CMFT(4.6)

Strangely enough, we can easily see that our coherent states diagonalize a_i irrespective of the choice we make of the scalar vector ϕ. We thus seem to have a (multiple) infinity of eigenstates, in other words: too many. In fact, coherent states form an (over)complete set of states in Fock space, and one should compensate for this overcompleteness by properly defining our resolution of the identity operator. The correct expression is

$$\int \prod_i \frac{d\bar{\phi}_i d\phi_i}{\pi} e^{-\sum_i \bar{\phi}_i\phi_i} |\phi\rangle\langle\phi| = \mathbf{1}_{\mathcal{F}} \tag{4.11}$$ CMFT(4.7)

with $d\bar{\phi}_i d\phi_i = d\Re\phi_i d\Im\phi_i$ and $\mathbf{1}_{\mathcal{F}}$ is the identity in Fock space. To prove this relation, it is sufficient to consider commuting it with any annihilation operator a_i: defining $d(\bar{\phi},\phi) \equiv \prod_i d\bar{\phi}_i d\phi_i/\pi$,

$$\begin{aligned} a_i\mathbf{1}_{\mathcal{F}} &= a_i \int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i}|\phi\rangle\langle\phi| = \int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i}\phi_i|\phi\rangle\langle\phi| \\ &= -\int d(\bar{\phi},\phi)(\partial_{\bar{\phi}_i} e^{-\sum_i \bar{\phi}_i\phi_i})|\phi\rangle\langle\phi| = \int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i}|\phi\rangle(\partial_{\bar{\phi}_i}\langle\phi|) \\ &= \int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i}|\phi\rangle\langle\phi|a_i = \mathbf{1}_{\mathcal{F}}\, a_i. \end{aligned} \tag{4.12}$$

Taking the adjoint of this then shows that the LHS of (4.11) also commutes with the set of creation operators. Since any state in Fock space can be obtained by summing a linear combination of (products of) creation operators acting on the vacuum, the LHS of (4.11) must thus indeed be proportional to identity operator. To compute this proportionality constant, one can simply consider the vacuum-vacuum matrix element

$$\int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i}\langle 0|\phi\rangle\langle\phi|0\rangle = \int d(\bar{\phi},\phi) e^{-\sum_i \bar{\phi}_i\phi_i} = 1. \tag{4.13}$$ CMFT(4.9)

where the last equality follows from (A.17).

4.1.2 Coherent states for fermions

Much of the coherent state formalism readily generalizes to fermions. In fact, the situation is in many aspects much simpler with fermions, though with a few peculiar features.

Let us thus being by supposing that our fermionic annihilation operators possess coherent states $|\eta\rangle$ such that

$$a_i|\eta\rangle = \eta_i|\eta\rangle \tag{4.14}$$ CMFT(4.10)

with η_i the eigenvalue. An important difference with the bosonic case (4.4) is that we now have to be consistent with the anti-commutativity of fermionic operators. Strangely enough, this means that to ensure consistency, the *eigenvalues* η_i have to anticommute[1],

$$\eta_i\eta_j = -\eta_j\eta_i, \qquad \forall i,j \tag{4.15}$$ CMFT(4.11)

[1] ... by which we here mean that they pick up a minus sign under interchange, not that they know anything about $\hbar$.

These thus cannot be ordinary numbers. In fact, we take η_i, $i = 1, ..., N$ to be the generators of a **Grassmann algebra** $\mathcal{A}$, their commutation relations being defined by (4.15). CMFT(4.11)

Remarkably, these numbers are even easier to do calculus with than the usual real or complex numbers.

The first important property of Grassmann numbers is that they are nilpotent, $\eta_i^2 = 0$. Functions of Grassmann numbers thus involve only the zeroth and first power of each generator, *e.g.* $f(\eta) = f(0) + f'(0)\eta$.

Differentiation is *defined* by the relation

$$\partial_{\eta_i}\eta_j = \delta_{ij} \tag{4.16}$$ CMFT(4.14)

Note that the differential operator must also be anticommuting to ensure consistency,

$$\partial_{\eta i}\partial_{\eta_j} = -\partial_{\eta_j}\partial_{\eta_i}. \tag{4.17}$$

A general function is thus defined via a Taylor expansion,

$$f(\xi_1, ..., \xi_k) = \sum_{n=0}^{\infty} \sum_{i_1,...,i_n=1}^{k} \frac{1}{n!} \frac{\partial^n f}{\partial\xi_{i_1}...\partial_{\xi_{i_n}}} \xi_{i_n}...\xi_{i_1}, \qquad \xi_1, ..., \xi_k \in \mathcal{A}. \tag{4.18}$$ CMFT(4.13)

Integration is *defined* symbolically as

$$\int d\eta_i = 0, \qquad \int d\eta_i \eta_i = 1. \tag{4.19}$$ CMFT(4.15)

You shouldn't think of this as a 'Riemann sum over Grassmann variables', but merely as an operator on elements of the Grassmann algebra. In fact, the remarkable this is that due to this definition, *Grassmann integration and differentiation are effectively identical*. Considering their action on a generic function of a single variable, we indeed see that

$$\int d\eta f(\eta) = \int d\eta (f(0) + f'(0)\eta) = f'(0) = \partial_\eta f(\eta). \tag{4.20}$$

The reason why we have introduced Grassmann variables is simply that they allow us to construct fermionic coherent states. For consistency, we first require that Grassmann numbers anticommute with fermion operators,

$$\{\eta_i, a_j\} = 0. \tag{4.21}$$ CMFT(4.16)

(note that by extension, we also require that the differential ∂_{η_i} and integration elements $d\eta_i$ anticommute with $a_i, a_i^\dagger$). It is then straightforward to see that

$$|\eta\rangle = \exp\left[-\sum_i \eta_i a_i^\dagger\right]|0\rangle \tag{4.22}$$ CMFT(4.17)

are **fermionic coherent states**. Checking explicitly,

$$\begin{aligned} a_i|\eta\rangle = \exp\left[-\sum_{j\neq i}\eta_j a_j^\dagger\right] a_i e^{-\eta_i a_i^\dagger}|0\rangle = \exp[...]a_i(1-\eta_i a_i^\dagger)|0\rangle \\ = \exp[...]\eta_i|0\rangle = \exp[...]\eta_i(1-\eta_i a_i^\dagger)|0\rangle = \eta_i|\eta\rangle. \end{aligned} \tag{4.23}$$

Taking the adjoint,

$$\langle\eta| = \langle 0| \exp\left[-\sum_i a_i\bar{\eta}_i\right] = \langle 0| \exp\left[\sum_i \bar{\eta}_i a_i\right]. \tag{4.24}$$

There exist a number of important differences between fermionic and bosonic coherent states:

1) the Grassmann vector elements $\bar{\eta}_i$ specifying the bra $\langle\eta|$ are *not* related to the η_i specifying $|\eta\rangle$ via some kind of (Grassmann) complex conjugation. They are instead to be seen as strictly independent variables.

2) The Grassmann version of the Gaussian integral is simply

$$\int d\bar{\eta}d\eta e^{-\bar{\eta}\eta} = \int d\bar{\eta}d\eta(1-\bar{\eta}\eta) = \int d\bar{\eta}(d\eta\eta)\bar{\eta} = \int d\bar{\eta}\bar{\eta} = 1 \tag{4.25}$$

and does *not* contain a factor of π like bosonic Gaussian integrals. The measure of the fermionic analogue of (CMFT(4.7) 4.11) does not contain π in the denominator.

To summarize, the definition and characteristics of bosonic and fermionic coherent states are (using our statistical factor $\zeta = \pm 1$ for bosons/fermions)

$$\begin{aligned}
\text{Definition} \qquad & |\psi\rangle = \exp\left[\zeta\sum_i \psi_i a_i^\dagger\right]|0\rangle && (4.26)\\
\text{Action of } a_i \qquad & a_i|\psi\rangle = \psi_i|\psi\rangle, \qquad \langle\psi|a_i = \partial_{\bar{\psi}_i}\langle\psi| && (4.27)\\
\text{Action of } a_i^\dagger \qquad & a_i^\dagger|\psi\rangle = \zeta\partial_{\psi_i}|\psi\rangle, \qquad \langle\psi|a_i^\dagger = \langle\psi|\bar{\psi}_i && (4.28)\\
\text{Overlap} \qquad & \langle\psi'|\psi\rangle = \exp\left[\sum_i \bar{\psi}'_i\psi_i\right] && (4.29)\\
\text{Completeness} \qquad & \int d(\bar{\psi},\psi)e^{-\sum_i\bar{\psi}_i\psi_i}|\psi\rangle\langle\psi| = \mathbf{1}_{\mathcal{F}}, && (4.30)\\
& d(\bar{\psi},\psi) = \begin{cases} \prod_i \frac{1}{\pi}d\Re\psi_i d\Im\psi_i, & \text{boson} \\ \prod_i d\bar{\psi}_i d\psi_i & \text{fermion} \end{cases}. && (4.31)
\end{aligned}$$

Exercise: show that (CMFT(4.3) 4.5), and (CMFT(4.4) 4.6), and (CMFT(4.5) 4.9), and (CMFT(4.6) 4.10) and (CMFT(4.7) 4.11) carry over to fermionic case.

• Show that $\langle\eta|a_i^\dagger = \langle\eta|\bar{\eta}_i$.

Answer:

$$\begin{aligned}
\langle\eta|a_i^\dagger &= \langle\eta|\exp\left[-\sum_j a_j\bar{\eta}_j\right]a_i^\dagger = \langle 0|\prod_j(1-a_j\bar{\eta}_j)a_i^\dagger = \langle 0|(1-a_i\bar{\eta}_i)a_i^\dagger\prod_{j\neq i}(1-a_j\bar{\eta}_j)\\
&= \langle 0|a_i a_i^\dagger\bar{\eta}_i\prod_{j\neq i}(1-a_j\bar{\eta}_j) = \langle 0|\prod_j(1-a_j\bar{\eta}_j)\bar{\eta}_i = \langle\eta|\bar{\eta}_i. \qquad (4.32)
\end{aligned}$$

• Show that $a_i^\dagger|\eta\rangle = -\partial_{\eta_i}|\eta\rangle$ and $\langle\eta|a_i = \partial_{\bar\eta_i}\langle\eta|$.

Answer:

$$\begin{aligned}
a_i^\dagger|\eta\rangle &= a_i^\dagger(1-\eta_i a_i^\dagger)\prod_{j\neq i}(1-\eta_j a_j^\dagger)|0\rangle = -\partial_{\eta_i}\prod_j(1-\eta_j a_j^\dagger)|0\rangle = -\partial_{\eta_i}|\eta\rangle.\\
\langle\eta|a_i &= \langle 0|\prod_{j\neq i}(1-a_j\bar\eta_j)(1-a_i\bar\eta_i)a_i = \langle 0|\prod_{j\neq i}(1-a_j\bar\eta_j)a_i\\
&= \langle 0|\prod_{j\neq i}(1-a_j\bar\eta_j)(-\partial_{\bar\eta_i}(a_i\bar\eta_i)) = \langle 0|\prod_{j\neq i}(1-a_j\bar\eta_j)\partial_{\bar\eta_i}(1-a_i\bar\eta_i)\\
&= \partial_{\bar\eta_i}\langle 0|\prod_j(1-a_j\bar\eta_j) = \partial_{\bar\eta_i}\langle\eta|. \qquad (4.33)
\end{aligned}$$

• Show that $\langle\eta|\nu\rangle = \exp\sum_i \bar\eta_i\nu_i$.

Answer:

$$\langle\eta|\nu\rangle = \langle\eta\prod_i(1-\nu_i a_i^\dagger)|0\rangle = \langle\eta|\prod_i(1+\bar\eta_i\nu_i)|0\rangle = \exp\sum_i \bar\eta_i\nu_i. \qquad (4.34)$$

• Show completeness. To prove this, show that the commutator of $a, a^\dagger$ operators with the resolution of the identity vanishes.

Answer:

$$\begin{aligned}
a_j^\dagger\ \mathbf{1}_{\mathcal{F}} &= a_j^\dagger\int d(\bar\eta,\eta)e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta| = -\int d(\bar\eta,\eta)e^{-\sum_i\bar\eta_i\eta_i}\partial_{\eta_j}|\eta\rangle\langle\eta|\\
&= \int d(\bar\eta,\eta)\partial_{\eta_j}e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta| = \int d(\bar\eta,\eta)\bar\eta_j e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta|\\
&= \int d(\bar\eta,\eta)e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta|a_j^\dagger = \mathbf{1}_{\mathcal{F}}\ a_j^\dagger.\\
a_j\ \mathbf{1}_{\mathcal{F}} &= \int d(\bar\eta,\eta)e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta| = \int d(\bar\eta,\eta)e^{-\sum_i\bar\eta_i\eta_i}\eta_j|\eta\rangle\langle\eta|\\
&= \int d(\bar\eta,\eta)(-\partial_{\bar\eta_j}e^{-\sum_i\bar\eta_i\eta_i})|\eta\rangle\langle\eta| = \int d(\bar\eta,\eta)e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\partial_{\bar\eta_j}\langle\eta|\\
&= \int d(\bar\eta,\eta)e^{-\sum_i\bar\eta_i\eta_i}|\eta\rangle\langle\eta|a_j = \mathbf{1}_{\mathcal{F}}\ a_j. \qquad (4.35)
\end{aligned}$$

Grassmann Gaussian integration Grassmann Gaussian integration obeys the simple identity

$$\int d\bar\eta d\eta e^{-\bar\eta a\eta} = a, \qquad a\in\mathbb{C}. \qquad (4.36)$$ CMFT(4.18)

Note that there is no issue of convergence here, irrespective of the value taken by the Gaussian parameter a.

This Grassmann Gaussian integral has the following multidimensional generalization:

$$\int d(\bar\phi,\phi)e^{-\bar\phi^T\mathbf{A}\phi} = \det\mathcal{A} \qquad (4.37)$$ CMFT(4.19)

where $\bar{\phi}$ and ϕ are N-component vectors of Grassmann variables, the measure is $d(\bar{\phi},\phi) \equiv \prod_{i=1}^{N} d\bar{\phi}_i d\phi_i$ and $\mathbf{A}$ can be an *arbitrary* complex matrix. Again, there is no convergence issue. The proof is left as an exercise.

Further useful identities are readily obtained. First, we can write the Grassmann version of (A.25): CMFT(3.18)

$$\int d(\bar{\phi},\phi) e^{-\bar{\phi}^T \mathbf{A}\phi + \bar{\nu}^T\cdot\phi + \bar{\phi}^T\cdot\nu} = \det \mathbf{A} e^{\bar{\nu}^T \mathbf{A}^{-1}\nu} \tag{4.38}$$

CMFT(4.22)

The proof is simple and uses the fact that Grassmann variables can be shifted in integrals: $\int d\eta f(\eta) = \int d\eta f(\eta+\nu)$.

Further integration formulas: define

$$\langle ... \rangle \equiv \det \mathbf{A}^{-1} \int d(\bar{\phi},\phi) e^{-\bar{\phi}^T \mathbf{A}\phi}(...), \tag{4.39}$$

one gets, by expanding both sides of (4.38), CMFT(4.22)

$$\int d(\bar{\phi},\phi) e^{-\bar{\phi}^T \mathbf{A}\phi}(... + \bar{\nu}_j \phi_j \bar{\phi}_i \nu_i + ...) = \det \mathbf{A}(... + \bar{\nu}_j A^{-1}_{ji} \nu_i + ...) \tag{4.40}$$

and therefore

$$\langle \phi_j \bar{\phi}_i \rangle = A^{-1}_{ji}. \tag{4.41}$$

This generalizes to

$$\langle \phi_{j_1}\phi_{j_2}...\phi_{j_n}\bar{\phi}_{i_n}...\bar{\phi}_{i_2}\bar{\phi}_{i_1}\rangle = \sum_P (-1)^P A^{-1}_{j_1 i_{P_1}}...A^{-1}_{j_n i_{P_n}}. \tag{4.42}$$

Connection between the path integral and statistical mechanics

For the moment: forget about QM, consider classical 1D continuum model of a flexible string, held under constant tension and confined to a 'gutter' potential. Assume that the mass density of the string is very high (kinetic energy is negligible). Transverse fluctuations: penalized by line tension and external potential. Assume that transverse displacement $u(x)$ is small.

Potential from line tension: $\delta V_{\text{tension}} = \sigma[(dx^2 + du^2)^{1/2} - dx] \simeq \sigma dx(\partial_x u)^2/2$. Integrating over length of string: $V_{\text{tension}}[\partial_x u] = \frac{1}{2}\int_0^L dx\sigma(\partial_x u(x))^2$.

Potential from external potential: $V_{\text{external}}[u] = \int_0^L dx V(u(x))$.

Total energy of string: $V = V_{\text{tension}} + V_{\text{external}} = \int_0^L dx[\frac{\sigma}{2}(\partial_x u)^2 + V(u)]$.

From general principles of stat mech: equilibrium properties encoded in partition function $\mathcal{Z} = \text{Tr}e^{-\beta V}$. Here, $\text{Tr} \to \int \mathcal{D}u$ so the partition function is

$$\mathcal{Z} = \int \mathcal{D}u \, \exp\left[-\beta \int_0^L dx \left(\frac{\sigma}{2}(\partial_x u)^2 + V(u)\right)\right]. \tag{4.43}$$

CMFT(3.22)

Comparing with (3.79),

CMFT(3.8)

$$\langle q_f|e^{-\frac{i}{\hbar}\hat{H}t}|q_i\rangle = \int \mathcal{D}q \, \exp\left[\frac{i}{\hbar}\int_0^t dt'(\frac{m}{2}\dot{q}^2 - V(q))\right] \tag{4.44}$$

CMFT(3.8bis)

with $L(q,\dot{q}) = \frac{m}{2}\dot{q}^2 - V(q)$: let $x' \in [0, L]$ be an **imaginary time** $x' = \tau' = it'$. We have $L = \tau = it$. Then,

$$\begin{aligned}\frac{i}{\hbar}\int_0^t dt'(\frac{m}{2}\dot{q}^2 - V(q))dt' &\to \frac{1}{\hbar}\int_0^{-i\tau} d\tau'(\frac{-m}{2}(\partial_{\tau'}q)^2 - V(q)) \\ &\to \frac{-1}{\hbar}\int_0^{\tau} d\tau'(\frac{\hat{p}^2}{2m} + V(q))\end{aligned} \tag{4.45}$$

where in the last step we have performed a **Wick rotation** of the integral interval by $\pi/2$ in the complex plane. Provided nothing goes wrong with this black magic, the partition function (4.43) of the classical system thus coincides with the quantum mechanical amplitude (4.44), evaluated at **imaginary time** $t = -i\tau \equiv -iL$ with $\hat{H} = \frac{\hat{p}^2}{2\sigma} + V(q)$ and we identify the tension with the mass, $\sigma = m$, and Planck's constant with the temperature, $\hbar = 1/\beta$.

CMFT(3.22)

CMFT(3.8bis)

This generalizes to higher dimensions: there is a close analogy between QFT in d dimensions and classical stat mech in $d+1$ dimensions.

Transformation $t \to -i\tau$ is called a **Wick rotation**. Imaginary time representations of Lagrangian actions are called **Euclidean**, whereas real time forms are **Minkowski** actions.

4.2 Field integral for the quantum partition function

According to the basic principles of (quantum) statistical mechanics, the finite temperature equilibrium physical propertires of a generic system are obtained from the **quantum partition function** (namely the trace in Fock space of the **Gibbs** distribution)

$$\mathcal{Z} = \text{ Tr } e^{-\beta(\hat{H}-\mu\hat{N})} = \sum_n \langle n|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle. \tag{4.46}$$ CMFT(4.23)

Here, $\beta = 1/T$ is the inverse temperature (we set $k_B = 1$), μ is the chemical potential, and sum over a complete set of states. For the moment, we don't yet specify whether we're working with fermions or not.

In addition to the partition function, we usually need to know **correlation functions**. Later on, we'll see that these can be obtained from a path integral similar to that for the partition function.

We begin by introducing a resolution of the identity in terms of coherent states:

$$\mathcal{Z} = \int d(\bar{\psi},\psi) e^{-\sum_i \bar{\psi}_i\psi_i} \sum_n \langle n|\psi\rangle\langle\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle. \tag{4.47}$$ CMFT(4.24)

Our next step is to get rid of redundant sum over $|n\rangle$. We here have to be a little bit careful with the (possibly Grassmann-valued) state overlaps and their sign changes upon reordering.

For bosons, we simply have: $\langle n|\psi\rangle\langle\psi|n\rangle = \langle\psi|n\rangle\langle n|\psi\rangle$.

For fermions, the general result is: $\langle n|\psi\rangle\langle\psi|n\rangle = \langle -\psi|n\rangle\langle n|\psi\rangle$ with $\langle -\psi| = \exp\,(-\sum_i \bar{\psi}_i a_i)$, since Grassmann variables anticommute with Fock space operators.

• **Exercise:** Show that $\langle n|\psi\rangle\langle\psi|n\rangle = \langle\zeta\psi|n\rangle\langle n|\psi\rangle$.

Answer: we have that $|n\rangle = a^\dagger_{i_1}..a^\dagger_{i_n}|0\rangle$ and $\langle n| = \langle 0|a_{i_n}...a_{i_1}$ (omitting normalization). Then,

$$\begin{aligned}
\langle n|\psi\rangle &= \langle 0|a_{i_n}...a_{i_1}|\psi\rangle = \langle 0|\psi_{i_n}...\psi_{i_1}|\psi\rangle = \psi_{i_n}...\psi_{i_1}. \\
\langle\psi|n\rangle &= \langle\psi|a^\dagger_{i_1}...a^\dagger_{i_n}|0\rangle = \langle\psi|\bar{\psi}_{i_1}...\bar{\psi}_{i_n}|0\rangle = \bar{\psi}_{i_1}...\bar{\psi}_{i_n}. \\
\langle n|\psi\rangle\langle\psi|n\rangle &= \psi_{i_n}...\psi_{i_1}\bar{\psi}_{i_1}...\bar{\psi}_{i_n} = \psi_{i_1}\bar{\psi}_{i_1}...\psi_{i_n}\bar{\psi}_{i_n} \\
&= (\zeta\bar{\psi}_{i_1}\psi_{i_1})...(\zeta\bar{\psi}_{i_n}\psi_{i_n}) = (\zeta\bar{\psi}_{i_1})...(\zeta\bar{\psi}_{i_n})\psi_{i_n}...\psi_{i_1} = \langle\zeta\psi|n\rangle\langle n|\psi\rangle.
\end{aligned} \tag{4.48}$$

Using our sign factor ζ (1 for bosons, -1 for fermions), the general expression is thus

$$\begin{aligned}
\mathcal{Z} &= \int d(\bar{\psi},\psi) e^{-\sum_i \bar{\psi}_i\psi_i} \sum_n \langle\zeta\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle\langle n|\psi\rangle \\
&= \int d(\bar{\psi},\psi) e^{-\sum_i \bar{\psi}_i\psi_i} \langle\zeta\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi\rangle.
\end{aligned} \tag{4.49}$$

This can now be used for constructing the path integral.

Let us assume that our Hamiltonian contains up to two-body terms only (as will be seen later, the generalization to higher-body terms is completely straightforward):

$$\hat{H}(a^\dagger,a) = \sum_{ij} h_{ij} a^\dagger_i a_j + \sum_{ijkl} V_{ijkl} a^\dagger_i a^\dagger_j a_k a_l. \tag{4.50}$$ CMFT(4.26)

This is a **normal ordered** form of the Hamiltonian. This will be crucial now: coherent states are eigenstates of the annihilation operators, and therefore (right-)diagonalize them all.

Following the path integral logic, let us now divide the (imaginary) time interval β into N segments and insert coherent state resolutions of the identity into (4.49) (see a more detailed derivation on the following page):

$$\mathcal{Z} = \int_{\bar\psi^0=\zeta\bar\psi^N,\psi^0=\zeta\psi^N} \prod_{n=0}^{N} d(\bar\psi^n,\psi^n) e^{-\delta\sum_{n=0}^{N-1}\left[\delta^{-1}(\bar\psi^n-\bar\psi^{n+1})\cdot\psi^n + H(\bar\psi^{n+1},\psi^n)-\mu N(\bar\psi^{n+1},\psi^n)\right]} \quad (4.51)$$

CMFT(4.27)

where $\delta=\beta/N$ and (similar equation for $N(\bar\psi,\psi')$)

$$\frac{\langle\psi|\hat H(a^\dagger,a)|\psi'\rangle}{\langle\psi|\psi'\rangle} = \sum_{ij} h_{ij}\bar\psi_i\psi'_j + \sum_{ijkl}\bar\psi_i\bar\psi_j\psi'_k\psi'_l \equiv H(\bar\psi,\psi').$$

Sending $N\to\infty$, and taking limits as for (3.74) and (3.77), we get the continuum version of the path integral:

$$\mathcal{Z} = \int \mathcal{D}(\bar\psi,\psi) e^{-S[\bar\psi,\psi]}, \qquad S[\bar\psi,\psi] = \int_0^\beta d\tau\left[\bar\psi\partial_\tau\psi + H(\bar\psi,\psi)-\mu N(\bar\psi,\psi)\right] \quad (4.52)$$

CMFT(3.5) CMFT(3.6) CMFT(4.28)

where $\mathcal{D}(\bar\psi,\psi)=\lim_{N\to\infty}\prod_{n=1}^N d(\bar\psi^n,\psi^n)$ and the fields satisfy the boundary conditions

$$\bar\psi(0)=\zeta\bar\psi(\beta), \qquad \psi(0)=\zeta\psi(\beta). \quad (4.53)$$

CMFT(4.29)

Written out explicitly, the action for Hamiltonian (4.50) is

$$S=\int_0^\beta d\tau\left[\sum_{ij}\bar\psi_i(\tau)\left[(\partial_\tau-\mu)\delta_{ij}+h_{ij}\right]\psi_j(\tau)+\sum_{ijkl}V_{ijkl}\bar\psi_i(\tau)\bar\psi_j(\tau)\psi_k(\tau)\psi_l(\tau)\right]. \quad (4.54)$$

CMFT(4.26) CMFT(4.30)

Equations (4.52) and (4.54) define the functional integral in the Euclidean time representation. A more practical rewriting is to use Fourier transformation from (imaginary) time to (imaginary) frequency,

$$\psi(\tau)=\frac{1}{\sqrt\beta}\sum_{\omega_n}\psi_n e^{-i\omega_n\tau}, \qquad \psi_n=\frac{1}{\sqrt\beta}\int_0^\beta d\tau\psi(\tau)e^{i\omega_n\tau},$$
$$\bar\psi(\tau)=\frac{1}{\sqrt\beta}\sum_{\omega_n}\bar\psi_n e^{i\omega_n\tau}, \qquad \bar\psi_n=\frac{1}{\sqrt\beta}\int_0^\beta d\tau\bar\psi(\tau)e^{-i\omega_n\tau},$$
$$\omega_n=\left\{\begin{array}{ll} 2n\pi T, & \text{bosons}\\ (2n+1)\pi T, & \text{fermions}\end{array}\right\} n\in\mathbb{Z} \quad (4.55)$$

the latter being known as the **Matsubara frequencies**, their quantization coming from the periodicity conditions (4.53).

CMFT(4.29)

Using this representation in (4.52) and (4.54), we get $\mathcal{Z}=\int\mathcal{D}(\bar\psi,\psi)e^{-S[\bar\psi,\psi]}$ with $\mathcal{D}(\bar\psi,\psi)=\prod_n d(\bar\psi_n,\psi_n)$ defining the measure. The action becomes

$$S[\bar\psi,\psi]=\sum_{ij,n}\bar\psi_{in}\left[(-i\omega_n-\mu)\delta_{ij}+h_{ij}\right]\psi_{jn}+\frac{1}{\beta}\sum_{ijkl,\{n_i\}}V_{ijkl}\bar\psi_{in_1}\bar\psi_{jn_2}\psi_{kn_3}\psi_{ln_4}\delta_{n_1+n_2,n_3+n_4} \quad (4.56)$$

CMFT(4.32)

where we have used $\int_0^\beta d\tau e^{-i(\omega_m-\omega_n)\tau}=\beta\delta_{m,n}$. This is the **frequency** representation of the action.

Recap of derivation of (4.27)

$$\mathcal{Z} = \int d(\bar{\psi},\psi) e^{-\sum_i \bar{\psi}_i \psi_i} \langle \zeta\psi | e^{-\beta(\hat{H}-\mu\hat{N})} | \psi \rangle \tag{4.57}$$

Resolution of identity:

$$\mathbf{1} = \int d(\bar{\psi},\psi) e^{-\sum_i \bar{\psi}_i \psi_i} |\psi\rangle\langle\psi| \tag{4.58}$$

Split β interval in N pieces:

$$e^{-\beta(\hat{H}-\mu\hat{N})} = e^{-\delta(\hat{H}-\mu\hat{N})}\mathbf{1}_{N-1} e^{-\delta(\hat{H}-\mu\hat{N})}\mathbf{1}_{N-2}...\mathbf{1}_1 e^{-\delta(\hat{H}-\mu\hat{N})} \tag{4.59}$$

so (writing the earlier ψ as ψ^0)

$$\mathcal{Z} = \int \prod_{n=0}^{N-1} d(\bar{\psi}^n,\psi^n) e^{-\sum_{n=0}^{N-1}\sum_i \bar{\psi}_i^n \psi_i^n} \langle \psi^N \equiv \zeta\psi^0 | e^{-\delta(\hat{H}-\mu\hat{N})} | \psi^{N-1}\rangle\langle\psi^{N-1}| e^{-\delta(\hat{H}-\mu\hat{N})}|\psi^{N-2}\rangle \times$$
$$\times \langle\psi^{N-2}|...|\psi^1\rangle\langle\psi^1|e^{-\delta(\hat{H}-\mu\hat{N})}|\psi^0\rangle \tag{4.60}$$

But

$$\langle\psi^{n+1}|e^{-\delta(\hat{H}-\mu\hat{N})}|\psi^n\rangle = e^{-\delta(H(\bar{\psi}^{n+1},\psi^n)-\mu N(\bar{\psi}^{n+1},\psi^n))}\langle\psi^{n+1}|\psi^n\rangle \tag{4.61}$$

and

$$\langle\psi^{n+1}|\psi^n\rangle = e^{\sum_i \bar{\psi}^{n+1}\psi^n} \tag{4.62}$$

so we get

$$\mathcal{Z} = \int_{\substack{\bar{\psi}^N = \zeta\bar{\psi}^0 \\ \psi^N = \zeta\psi^0}} \prod_{n=0}^{N-1} d(\bar{\psi}^n,\psi^n) \exp\left\{ -\sum_{n=0}^{N-1}(\bar{\psi}_i^n - \bar{\psi}_i^{n+1})\psi_i^n - \delta\sum_{n=0}^{N-1}[H(\bar{\psi}^{n+1},\psi^n) - \mu N(\bar{\psi}^{n+1},\psi^n)]\right\} \tag{4.63}$$

Defining $\partial_\tau\bar{\psi} \equiv \bar{\psi}_i^{n+1} - \bar{\psi}_i^n$ and $\mathcal{D}(\bar{\psi},\psi) = \lim_{N\to\infty}\prod_{n=0}^{N-1} d(\bar{\psi}^n,\psi^n)$, we arrive (after a simple partial integration in τ, and neglecting higher-order differentials in the limit $N\to\infty$) to the final form of the imaginary-time functional field integral:

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}(\bar{\psi},\psi) e^{-S[\bar{\psi},\psi]}, \\ S[\bar{\psi},\psi] &= \int_0^\beta d\tau \left[\sum_i \bar{\psi}_i(\tau)\partial_\tau\psi_i(\tau) + H(\bar{\psi}(\tau),\psi(\tau)) - \mu N(\bar{\psi}(\tau),\psi(\tau))\right]. \end{aligned} \tag{4.64}$$

4.2.1 Partition function of the noninteracting gas

Consider (4.52) with

$$H_0(\bar\psi,\psi)=\sum_{i,j}\bar\psi_i H_{0,ij}\psi_j. \tag{4.65}$$

Diagonalize H_0 by unitary transformation U, $H_0 = UDU^\dagger$, $D = \mathrm{diag}(\varepsilon_1,...)$. Change integration variables $U^\dagger\psi\equiv\phi$. Action becomes

$$S=\sum_a\sum_{\omega_n}\bar\phi_{an}(-i\omega_n+\xi_a)\phi_{an},\qquad \xi_a\equiv\varepsilon_a-\mu. \tag{4.66}$$

The partition function decouples,

$$\mathcal{Z}=\prod_a\mathcal{Z}_a \tag{4.67}$$

with

$$\mathcal{Z}_a=\int\mathcal{D}(\bar\phi_a,\phi_a)e^{-\sum_n\bar\phi_{an}(-i\omega_n+\xi_a)\phi_{an}}=\prod_n\left[\beta(-i\omega_n+\xi_a)\right]^{-\zeta}. \tag{4.68}$$

CMFT(4.33)

The free energy is thus a simple sum,

$$\mathcal{F}=-T\ln\mathcal{Z}=T\zeta\sum_{a,n}\ln\left[\beta(-i\omega_n+\xi_a)\right]. \tag{4.69}$$

CMFT(4.34)

Matsubara frequency summations Summations like the one in (4.69) are frequently encountered in this business. There is a standard trick to perform them. Consider a single Matsubara sum of some function,

$$S\equiv\sum_{\omega_n}h(\omega_n). \tag{4.70}$$

CMFT(4.36)

The basic idea is to introduce an auxiliary function $g(z)$ having simple poles at all $z=i\omega_n$. The Matsubara sum is then transformed into a sum over residues of hg.

Two common choices for g (infinitely many choices are possible) are:

$$g(z)=\begin{cases}\frac{\beta}{e^{\beta z}-1}, & \text{bosons}\\ \frac{\beta}{e^{\beta z}+1}, & \text{fermions}\end{cases}\qquad g(z)=\begin{cases}\frac{\beta}{2}\coth\frac{\beta z}{2}, & \text{bosons}\\ \frac{\beta}{2}\tanh\frac{\beta z}{2}, & \text{fermions}\end{cases}. \tag{4.71}$$

CMFT(4.37)

Explicit check: for bosons, $g(z)=\frac{\beta}{e^{\beta z}-1}$ around $z=i\omega_n=i\frac{2\pi n}{\beta}$ goes like $\beta[e^{\beta(z-i\omega_n)+\beta i\omega_n}-1]^{-1}=\beta[e^{\beta(z-\imath\omega_n)}-1]^{-1}\simeq\frac{1}{z-i\omega_n}$ so we get a simple pole with residue factor 1. For fermions, $g(z)=\frac{\beta}{e^{\beta z}+1}$ around $z=i\omega_n=i\frac{(2n+1)\pi}{\beta}$ goes like $\beta[e^{\beta(z-i\omega_n)+\beta i\omega_n}+1]^{-1}=-\beta[e^{\beta(z-\imath\omega_n)}-1]^{-1}\simeq\frac{-1}{z-i\omega_n}$ so we get a simple pole with residue factor -1.

Consider now integrating hg along the contour γ_1 (see figure 4.1, left)

fig:Matsubara_gamma

fig:Matsubara_gamma

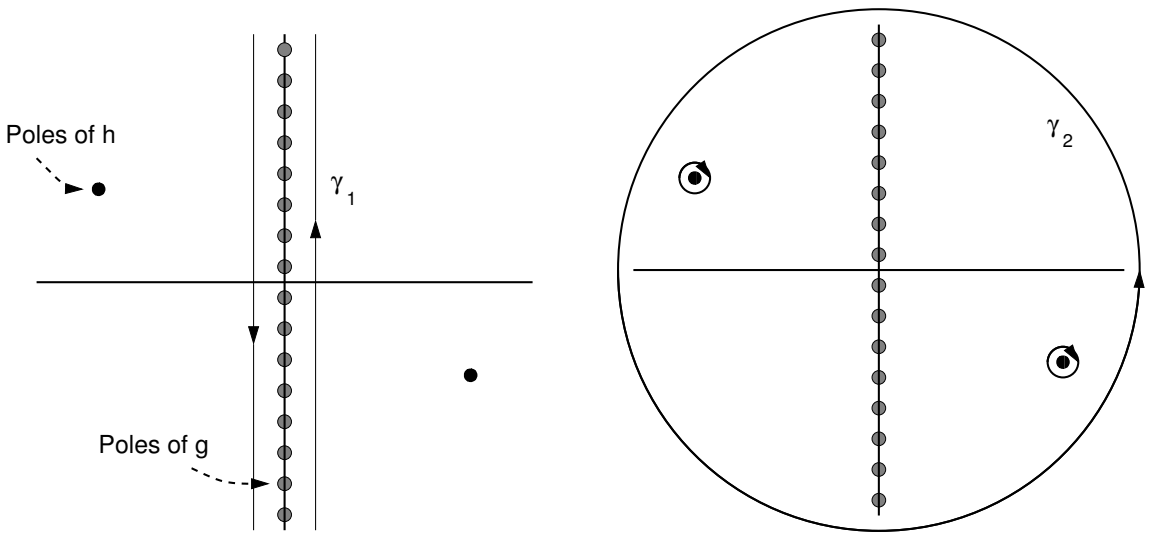

Figure 4.1: Left: γ_1 contour. Right: γ_2 contour, obtained after expanding.

We have on the one hand that

$$\frac{\zeta}{2\pi i}\oint_{\gamma_1} dz g(z)h(-iz) = \zeta\sum_n \text{ Res } [g(z)h(-iz)]|_{z=i\omega_n} = \sum_n h(\omega_n) = S. \tag{4.72}$$

We can however inflate the γ_1 contour towards infinity. In the case where $h(-iz)$ has isolated singularities at the set of points $\{z_k\}$, this yields the new γ_2 contour (see figure 4.1, right) composed of a contour at infinity with additional contributions from the poles of h. If the contour at infinity has vanishing contribution, we therefore obtain

fig:Matsubara_gamma

$$S = \frac{\zeta}{2\pi i}\oint_{\gamma_2} dz h(-iz)g(z) = -\zeta\sum_k \text{ Res } [h(-iz)g(z)]_{z=z_k} \tag{4.73}$$

CMFT(4.38)

so the infinite sum over Matsubara frequencies becomes a sum (often finite) over residues at poles of the h function.

Example: let $h(\omega_n) = \frac{-\zeta T}{i\omega_n e^{-i\omega_n\delta}-\xi}$ with some regulator $\delta > 0$. The product $h(-iz)g(z)$ decays to 0 at $|z| \to \infty$. $h(-iz)$ has a simple pole at $z = \xi$ (for $\delta \to 0$). Thus,

$$\sum_n h(\omega_n) = -\zeta \text{ Res}[g(z)h(-iz)]|_{z=\xi} = -\zeta\frac{\beta}{e^{\beta\xi}-\zeta}(-\zeta T) = \frac{1}{e^{\beta\xi}-\zeta} \tag{4.74}$$

so we get

$$-\zeta T\sum_n \frac{1}{i\omega_n - \xi_a} = \begin{cases} n_B(\varepsilon_a), & \text{bosons} \\ n_F(\varepsilon_a), & \text{fermions} \end{cases} \tag{4.75}$$

CMFT(4.39)

with

$$n_B(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}-1}, \qquad n_F(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1} \tag{4.76}$$

CMFT(4.40)

being the bosonic and fermionic occupation factors respectively.

We can also look at the free energy $\mathcal{F}$ itself. For that, we have $h(\omega_n) = \zeta T \ln[\beta(-i\omega_n + \xi)]$. The function $h(-iz) = \zeta T \ln(\xi - z)$ has a branch cut along the real axis on the interval $[\xi, \infty[$. The contour thus needs to be bent as in figure 4.2, fig:Matsubara_for_F

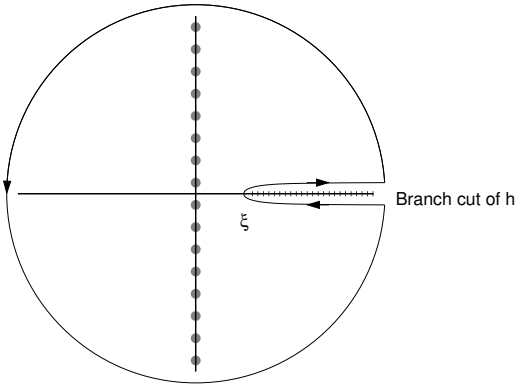

Figure 4.2: Matsubara contour for the free energy of the noninteracting gas.

fig:Matsubara_for_F

so we can write (choosing $g(z) = \frac{\beta}{e^{\beta z} - \zeta}$)

$$S = \frac{T}{2\pi i}\left(\int_{\xi}^{\infty} dz g(z) \ln[\xi - z - i\delta] + \int_{\infty}^{\xi} dz g(z) \ln[\xi - z + i\delta]\right)$$
$$= \frac{T}{2\pi i}\int_{-\infty}^{\infty} dz g(z) \left(\ln[\xi - z - i\delta] - \ln[\xi - z + i\delta]\right). \tag{4.77}$$

Using the fact that $g(z) = \frac{\beta}{e^{\beta z} - \zeta} = \zeta \partial_z \ln(1 - \zeta e^{-\beta z})$ and integrating by parts (boundary terms vanish), we get

$$S = -\frac{\zeta T}{2\pi i}\int_{-\infty}^{\infty} dz \ln(1 - \zeta e^{-\beta z})\left(\frac{1}{z - \xi + i\delta} - \frac{1}{z - \xi - i\delta}\right). \tag{4.78}$$

Now use identity (see (CMFT(3.58))) $\frac{1}{x + i\delta} = -i\pi\delta(x) + \mathcal{P}\frac{1}{x}$ to obtain

$$S = \zeta T \ln[1 - \zeta e^{-\beta\xi}] \tag{4.79}$$

so that the full free energy finally reads

$$\mathcal{F} = \zeta T \sum_a \ln[1 - \zeta e^{-\beta\xi_a}] \tag{4.80}$$ CMFT(4.41)

which is the familiar expression CMFT(4.34)

From our free energy (4.69), we can for example now calculate the particle number:

$$N = -\frac{\partial \mathcal{F}}{\partial \mu} = -\frac{\partial}{\partial \mu} T\zeta \sum_{an} \ln\left[\beta(-i\omega_n + \xi_a)\right]. \tag{4.81}$$

Using $\partial\xi/\partial\mu = -1$ immediately yields

$$N = T\zeta \sum_{an} \frac{1}{-i\omega_n + \xi_a} = \sum_a n_{B,F}(\varepsilon_a). \tag{4.82}$$

Problem 4.5.6 Pauli paramagnetism

$$\hat{H}_z = -\mu_0 \mathbf{B}\cdot\hat{\mathbf{S}}, \qquad \hat{\mathbf{S}} = \sum_{\alpha\sigma\sigma'} \frac{1}{2} a^\dagger_{\alpha\sigma}\sigma_{\sigma\sigma'}a_{\alpha\sigma'} \tag{4.83}$$

Here, α is an orbital quantum number and $\mu_0 = e/2m$ is the Bohr magneton.

Two-fold spin degenerate single-particle band of free electron states. Both bands are filled up to chemical potential μ. Switching on of external field: degeneracy lifted, two bands shift in opposite directions.

a) coherent state action Consider $\hat{H} = \hat{H}_0 + \hat{H}_z$ with $\hat{H}_0 = \sum_{\alpha,\sigma} a^\dagger_{\alpha\sigma}\varepsilon_\alpha a_{\alpha\sigma}$ the non-magnetic part of Hamiltonian. Integrate out the Grassmann fields to obtain the free energy F as a sum over frequencies.

Answer : using quantization along field axis,

$$\hat{H} = \sum_{\alpha\sigma} a^\dagger_{\alpha\sigma}\left[\frac{p^2}{2m} - \frac{\mu_0 B}{2}(\sigma^z)_{\sigma\sigma}\right] a_{\alpha\sigma} \tag{4.84}$$

Action: use (CMFT(4.32) 4.56), with $h_{ij} = \varepsilon_i\delta_{ij}$ and $V_{ijkl} = 0$. Denoting $\varepsilon_\alpha - \mu = \xi_\alpha$,

$$S[\bar{\psi},\psi] = \sum_{\alpha\sigma n} \bar{\psi}_{\alpha\sigma n}\left[-i\omega_n + \xi_\alpha - \frac{\mu_0 B}{2}(\sigma^z)_{\sigma\sigma}\right]\psi_{\alpha\sigma n} \tag{4.85}$$

Integrating over ψ (keep in mind normalization of measure, as per footnote 11 on p.169 of CMFT: $d(\bar{\psi}_n,\psi_n) = \beta d\bar{\psi}_n d\psi_n$ (F), $d(\bar{\psi}_n,\psi_n) = \frac{1}{\pi\beta} d\bar{\psi}_n d\psi_n$ (B), so that $\int d(\bar{\psi}_n,\psi_n) e^{-\bar{\psi}_n\varepsilon\psi_n} = (\beta\varepsilon)^{-\zeta}$).

$$\begin{aligned}
\mathcal{Z} = \int \mathcal{D}(\bar{\psi},\psi) e^{-S[\bar{\psi},\psi]} &= \prod_{\alpha\sigma n}\int d(\bar{\psi}_{\alpha\sigma n},\psi_{\alpha\sigma n})\ \exp\left[-\bar{\psi}_{\alpha\sigma n}\left(-i\omega_n + \xi_\alpha - \frac{\mu_0 B}{2}\sigma\right)\psi_{\alpha\sigma n}\right] \\
&= \prod_{\alpha\sigma n}\left[\beta(-i\omega_n + \xi_\alpha - \frac{\mu_0 B}{2}\sigma)\right] = \prod_{\alpha n}\left[\beta^2\left[(-i\omega_n+\xi_\alpha)^2 - \frac{\mu_0^2 B^2}{4}\right]\right], \\
F = -T\ln\mathcal{Z} &= -T\sum_{\alpha,n}\ln\left[\beta^2\left[(-i\omega_n+\xi_\alpha)^2 - \frac{\mu_0^2 B^2}{4}\right]\right]
\end{aligned} \tag{4.86}$$

b) low-temperature susceptibility The magnetization is given by the derivative of the free energy w/r to the field, $M = \partial_B F$. The susceptibility is the rate of change of magnetization w/r to field at zero field, so

$$\chi \equiv -\partial_B^2 F|_{B=0} \tag{4.87}$$

First derivative:

$$\begin{aligned}
\partial_B F &= T\frac{\mu_0^2 B}{2}\sum_{\alpha n}\left[(-i\omega_n+\xi_\alpha)^2 - \frac{\mu_0^2 B^2}{4}\right]^{-1}, \\
\chi &= -\frac{\mu_0^2 T}{2}\sum_{\alpha n}(-i\omega_n+\xi_\alpha)^{-2} \equiv \sum_{\alpha n} h_\alpha(\omega_n).
\end{aligned} \tag{4.88}$$

The function $h_\alpha(-iz) = -\frac{\mu_0^2 T}{2}\frac{1}{(-z+\xi_\alpha)^2}$ has a pole of second order at ξ_α. We can now use (4.73): CMFT(4.38)

$$\text{Res } [h(-iz)g(z)]|_{z=\xi_\alpha} = -\frac{\mu_0^2 T}{2} g'(\xi_\alpha) = -\frac{\mu_0^2 T}{2}\frac{-\beta^2 e^{\beta\xi_\alpha}}{(e^{\beta\xi_\alpha}+1)^2} = -\frac{\mu_0^2}{2} n'_F(z)|_{z=\xi_\alpha}$$

$$\chi = -\zeta \sum_\alpha \text{ Res } [h(-iz)g(z)]_{z=\xi_\alpha} = -\frac{\mu_0^2}{2}\sum_\alpha n'_F(\xi_\alpha) = -\frac{\mu_0^2}{2}\int_{-\infty}^{\infty} d\varepsilon \rho(\varepsilon) n'_F(\varepsilon-\mu). \quad (4.89)$$

Since $\lim_{T\to 0} n_F(\varepsilon) = \theta(-\varepsilon)$, we have $\lim_{T\to 0} n'_F(\varepsilon) = -\delta(\varepsilon)$ so

$$\chi \to_{T\to 0} \frac{\mu_0^2}{2}\rho(\mu). \quad (4.90)$$

4.5.7 Electron-phonon coupling

$$\hat{H}_{ph} = \sum_{\mathbf{q}j} \omega_q a^\dagger_{\mathbf{q}j} a_{\mathbf{q}j} + cst. \tag{4.91}$$

Phonon dispersion relation depends only on modulus $|\mathbf{q}| = q$, index j refers to three possible phonon oscillations in space.

Electrons in medium: sense induced charge $\rho_{ind} \sim \nabla \cdot \mathbf{P}$ where $\mathbf{P} \sim \mathbf{u}$ is the polarization generated by local distortion $\mathbf{u}$ of the lattice ($\mathbf{u}(\mathbf{r})$ is the 3d displacement). In terms of phonon creation and annihilation operators (see (1.40)),

$$u(\mathbf{r}) = \frac{1}{L^{d/2}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} u_{\mathbf{q}}, \qquad \mathbf{u}_{\mathbf{q}} = \frac{\mathbf{e}_j}{(2m\omega_q)^{1/2}} (a_{\mathbf{q},j} + a^\dagger_{-\mathbf{q},j}) \tag{4.92}$$

with $\mathbf{e}_j$ the unit vector in direction j.

Electron-phonon Hamiltonian:

$$\begin{aligned} \hat{H}_{el-ph} = \gamma \int d^d r \hat{n}(\mathbf{r}) \nabla \cdot \mathbf{u}(\mathbf{r}) &= \gamma \int \frac{d^d r}{L^d} \sum_{\mathbf{q}_1, \mathbf{q}_2} n_{\mathbf{q}_1} u_{\mathbf{q}_2} e^{i(\mathbf{q}_1+\mathbf{q}_2)\cdot\mathbf{r}} \sum_j i q_{2,j} \\ &= \gamma \sum_{\mathbf{q},j} \frac{i q_j}{(2m\omega_q)^{1/2}} \hat{n}_{-\mathbf{q}} (a_{\mathbf{q},j} + a^\dagger_{-\mathbf{q},j}) \end{aligned} \tag{4.93}$$

with $\hat{n}(\mathbf{r}) = c^\dagger(\mathbf{r}) c(\mathbf{r})$ the number operator, whose Fourier transform (using $c(\mathbf{r}) = \frac{1}{L^{d/2}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} c_{\mathbf{q}}$)

$$\hat{n}_{\mathbf{q}} = \frac{1}{L^{d/2}} \int d^d r e^{i\mathbf{q}\cdot\mathbf{r}} \hat{n}(\mathbf{r}) = \frac{1}{L^{3d/2}} \sum_{\mathbf{q}_1, \mathbf{q}_2} c^\dagger_{\mathbf{q}_1} c_{\mathbf{q}_2} \underbrace{\int d^d r e^{i(\mathbf{q}-\mathbf{q}_1+\mathbf{q}_2)\cdot\mathbf{r}}}_{L^d \delta_{\mathbf{q}_1-\mathbf{q}_2,\mathbf{q}}} = \frac{1}{L^{d/2}} \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \tag{4.94}$$

is the electronic density in Fourier space (we neglect spin for simplicity).

a) Formulate the coherent state action. Introduce Grassmann field ψ for electrons, and complex ϕ for phonons. Coherent state PI:

$$\begin{aligned} \mathcal{Z} = \int \mathcal{D}[\bar{\psi}, \psi] \int \mathcal{D}[\bar{\phi}, \phi] \, \exp\, \left[-S_{el}[\bar{\psi}, \psi] - S_{ph}[\bar{\phi}, \phi] - S_{el-ph}[\bar{\psi}, \psi, \bar{\phi}, \phi] \right], \\ S_{ph}[\bar{\phi}, \phi] = \sum_{\mathbf{q},n,j} \bar{\phi}_{\mathbf{q}nj} (-i\omega_n + \omega_q) \phi_{\mathbf{q}nj}, \\ S_{el-ph}[\bar{\psi}, \psi, \bar{\phi}, \phi] = \gamma \sum_{\mathbf{q}nj} \frac{i q_j}{(2m\omega_q)^{1/2}} \rho_{-\mathbf{q}-n} (\phi_{\mathbf{q}nj} + \bar{\phi}_{-\mathbf{q}-nj}), \end{aligned} \tag{4.95}$$

with $\rho_{\mathbf{q}} = \frac{1}{L^{d/2}} \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}+\mathbf{q}} \psi_{\mathbf{k}}$.

b) Integrate out the phonon fields and show that an attractive interaction between electrons is generated. Effective action:

$$\int \mathcal{D}[\bar{\phi},\phi] e^{-S_{\text{ph}}[\bar{\phi},\phi]-S_{\text{el-ph}}[\bar{\psi},\psi,\bar{\phi},\phi]} =$$

$$= \int \mathcal{D}[\bar{\phi},\phi] \exp\left\{-\sum_{\mathbf{q}nj}\bar{\phi}_{\mathbf{q}nj}(-i\omega_n+\omega_q)\phi_{\mathbf{q}nj} - \gamma\sum_{\mathbf{q}nj}\frac{iq_j}{(2m\omega_q)^{1/2}}\rho_{-\mathbf{q}-n}(\phi_{\mathbf{q}nj}+\bar{\phi}_{-\mathbf{q}-nj})\right\}$$

$$= \int \mathcal{D}[\bar{\phi},\phi] \exp\left\{-\sum_{\mathbf{q}nj}\left[\bar{\phi}_{\mathbf{q}nj}(-i\omega_n+\omega_q)\phi_{\mathbf{q}nj} + \frac{i\gamma q_j}{(2m\omega_q)^{1/2}}\left(\rho_{-\mathbf{q}-n}\phi_{\mathbf{q}nj} - \bar{\phi}_{\mathbf{q}nj}\rho_{\mathbf{q}n}\right)\right]\right\}$$

$$= \prod_{\mathbf{q}nj}\int d(\bar{\phi}_{\mathbf{q}nj},\phi_{\mathbf{q}nj}) \exp\left\{-\left[\bar{\phi}_{\mathbf{qnj}} - \frac{i\gamma q_j}{(2m\omega_q)^{1/2}}\frac{\rho_{-\mathbf{q}-n}}{-i\omega_n+\omega_q}\right]\times\right.$$

$$\left.\times(-i\omega_n+\omega_q)\left[\phi_{\mathbf{qnj}} + \frac{i\gamma q_j}{(2m\omega_q)^{1/2}}\frac{\rho_{\mathbf{q}n}}{-i\omega_n+\omega_q}\right]\right\}\times \exp\left\{\frac{\gamma^2 q_j^2}{2m\omega_q}\frac{1}{-i\omega_n+\omega_q}\rho_{\mathbf{q}n}\rho_{-\mathbf{q}-n}\right\}$$

$$= \exp\left\{\frac{\gamma^2}{2m}\sum_{\mathbf{q}n}\frac{q^2}{\omega_q}\frac{1}{-i\omega_n+\omega_q}\rho_{\mathbf{q}n}\rho_{-\mathbf{q}-n}\right\} \tag{4.96}$$

so the effective action for the electrons becomes

$$S_{\text{eff}}[\bar{\psi},\psi] = S_{\text{el}}[\bar{\psi},\psi] - \frac{\gamma^2}{2m}\sum_{\mathbf{q}n}\frac{q^2}{\omega_q}\frac{1}{-i\omega_n+\omega_q}\rho_{\mathbf{q}n}\rho_{-\mathbf{q}-n}. \tag{4.97}$$

Only the symmetric term survives: $\frac{1}{-i\omega_n+\omega_q} \to_{\sum} \frac{\omega_q}{\omega_n^2+\omega_q^2}$ so we can write

$$S_{\text{eff}}[\bar{\psi},\psi] = S_{\text{el}}[\bar{\psi},\psi] - \frac{\gamma^2}{2m}\sum_{\mathbf{q}n}\frac{q^2}{\omega_n^2+\omega_q^2}\rho_{\mathbf{q}n}\rho_{-\mathbf{q}-n}. \tag{4.98}$$

Chapter 5

Perturbation theory

PT

5. Perturbation theory

5.1 General structure of low-order expansions

5.1.1 Example integral

Consider

$$I(g) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2} - g x^4}. \tag{5.1}$$

CMFT(5.1)

This is like a particle in a harmonic potential, with an anharmonic correction. For small $g \ll 1$, we can try to expand in g:

$$I(g) = \sum_{n=0}^{\infty} g^n I_n, \qquad g^n I_n = \frac{(-g)^n}{n!} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} x^{4n}. \tag{5.2}$$

But we know from our Gaussian integrals that

$$I(a) \equiv \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-\frac{a x^2}{2}} = \frac{1}{\sqrt{a}}, \qquad \langle x^2 \rangle_a = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-\frac{a x^2}{2}} x^2 = -2 \frac{d}{da} I(a) = \frac{1}{a^{3/2}},$$
$$\langle x^4 \rangle_a = 4 \frac{d^2}{da^2} I(a) = \frac{3}{a^{5/2}}, ... \qquad \langle x^{4n} \rangle = 2^{2n} \frac{d^{2n}}{da^{2n}} I(a)|_{a=1} = (4n-1)(4n-3)... = (4n-1)!! \tag{5.3}$$

so

$$g^n I_n = (-g)^n \frac{(4n-1)!!}{n!} \simeq (-g)^n \frac{[(4n)^{4n} e^{-4n}]^{1/2}}{n^n e^{-n}} \simeq (-(cst) \frac{gn}{e})^n. \tag{5.4}$$

Problem: expansion in g small does not exist ! Series begins to diverge around order $n \sim 1/g$.

N.B.: what is the radius of convergence in g ? $g > 0$: $I(g)$ converges. $g < 0$: $I(g)$ is divergent ! Therefore, the radius of convergence is 0!

More 'physical' picture: use (CMFT(3.16) A.23),

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} x^{4n} = \sum_{\text{all pairings}} 1 = (4n-1)!! \tag{5.5}$$

Perturbative breakdown of expansion: competition between smallness of g and proliferating number of 'interaction pairings'.

All is not lost, however. Infinite series is divergent, but *partial resummation* $I_{n_{max}}(g) \equiv \sum_{n=0}^{n_{max}} g^n I_n$ can give an excellent approximation to $I(g)$. To see this: estimate the error

$$\left| I(g) - \sum_{n=0}^{n_{max}} g^n I_n \right| \leq g^{n_{max}+1} |I_{n_{max}+1}| \sim (\frac{g n_{max}}{e})^{n_{max}}. \tag{5.6}$$

Vary with respect to $n_{max} \equiv n$:

$$e^{n \ln g + n \ln n - n} \to \frac{d}{dn}(...) = \ln g + \ln n = 0 \to n_{opt} \sim 1/g \tag{5.7}$$

so the error is optimized for $n_{max} \sim 1/g$. Making this choice, the error scales as $e^{-1/g}$. For $g = 0.01$: error is of scale $e^{-100} \sim 10^{-30}$. For $g = 0.3$, scale is e^{-3}. Then, perturbation theory is bad already at about third order !

Message: perturbative expansions **are not** rigorous Taylor expansions. Rather, they are **asymptotic expansions**.

5.1.2 ϕ^4 theory

Simplest interacting field theory:

$$\mathcal{Z} = \int \mathcal{D}\phi e^{-S[\phi]}, \qquad S[\phi] = \int d^d x \left[\frac{1}{2}(\partial\phi)^2 + \frac{m^2}{2}\phi^2 + g\phi^4\right] \tag{5.8}$$ CMFT(5.2)

Appears in many applications:

1. d-dimensional Ising model close to critical point
2. more generally: classical stat. mech. systems with a scalar order parameter: $S[\phi]$ is the Ginzburg-Landau free energy functional.

Nomenclature for perturbation theory:

$$\langle ... \rangle \equiv \frac{\int \mathcal{D}\phi(...)e^{-S[\phi]}}{\int \mathcal{D}\phi e^{-S[\phi]}} \tag{5.9}$$ CMFT(5.6)

is called the **functional average** or **expectation value** of (...). Similarly, the free average is defined as

$$\langle ... \rangle_0 \equiv \frac{\int \mathcal{D}\phi(...)e^{-S_0[\phi]}}{\int \mathcal{D}\phi e^{-S_0[\phi]}}, \qquad S_0[\phi] \equiv S[\phi]|_{g=0}. \tag{5.10}$$ CMFT(5.7)

Average over product of field variables:

$$C_n(\mathbf{x}_1, ..., \mathbf{x}_n) \equiv \langle \phi(\mathbf{x}_1)...\phi(\mathbf{x}_n) \rangle \tag{5.11}$$

is the **n-point correlation function** of the field ϕ. The simplest function is the one-point function $C_1(\mathbf{x}) = \langle \phi(\mathbf{x}) \rangle$ which corresponds to the field's expectation value. For field theories which have only even-power terms, this vanishes.

The first truly nontrivial function is the two-point function

$$\mathcal{G}(\mathbf{x}_1 - \mathbf{x}_2) \equiv C_2(\mathbf{x}_1, \mathbf{x}_2) \tag{5.12}$$

which is called the **propagator** or **Green function** (here, we assumed translational invariance; this is not always the case !).

Dimensional analysis. The action itself is a dimensionless number. Simple inspection gives

$$L^{d-2}[\phi]^2 = 1, \quad L^d[m]^2[\phi]^2 = 1, \quad L^d[g][\phi]^4 = 1 \tag{5.13}$$

and thus

$$[\phi] = L^{-(d-2)/2}, \quad [m] = L^{-1}, \quad [g] = L^{d-4}. \tag{5.14}$$

The 'mass' parameter thus represents an inverse length scale; this length scale sets the correlation length (at least in the unperturbed theory).

Propagator for the Gaussian model (free bosonic field) Use FT:

$$\phi(\mathbf{x}) = \frac{1}{L^{d/2}} \sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot\mathbf{x}} \phi_{\mathbf{p}} \tag{5.15}$$

Action becomes

$$S_0[\phi] = \sum_{\mathbf{p}} \frac{1}{2}\phi_{\mathbf{p}}(p^2+m^2)\phi_{-\mathbf{p}}. \tag{5.16}$$

Consider now

$$\mathcal{G}_0(\mathbf{x}) \equiv \langle \phi(\mathbf{x})\phi(0)\rangle_0. \tag{5.17}$$

CMFT(5.10)

This is

$$\mathcal{G}_0(\mathbf{x}) = \frac{1}{L^d}\sum_{\mathbf{p},\mathbf{p}'} e^{-i\mathbf{p}\cdot\mathbf{x}}\langle \phi_{\mathbf{p}}\phi_{\mathbf{p}'}\rangle_0 \tag{5.18}$$

CMFT(3.14)

Using the Gaussian contraction rule (A.20) and defining the FT of the propagator

$$\langle \phi_{\mathbf{p}}\phi_{\mathbf{p}'}\rangle_0 = \delta_{\mathbf{p}+\mathbf{p}',0}\frac{1}{p^2+m^2}, \qquad \mathcal{G}_{0,\mathbf{p}} = \langle \phi_{\mathbf{p}}\phi_{-\mathbf{p}}\rangle_0 = \frac{1}{p^2+m^2}, \tag{5.19}$$

we get the real-space propagator:

$$\mathcal{G}_0(\mathbf{x}) = \frac{1}{L^d}\sum_{\mathbf{p}} e^{-i\mathbf{p}\cdot\mathbf{x}}\mathcal{G}_{0,\mathbf{p}} \quad \underset{L\to\infty}{\longrightarrow} \quad \int \frac{d^dp}{(2\pi)^d}\frac{e^{-i\mathbf{p}\cdot\mathbf{x}}}{p^2+m^2}. \tag{5.20}$$

Note that the propagator solves the equation

$$(-\partial_{\mathbf{r}}^2 + m^2)G(\mathbf{r}-\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \tag{5.21}$$

which is why we call it the Green's function (or resolvent) of this kernel.

5.1.3 Perturbation theory at low orders

We now need to deal with the interaction part of the action:

$$S_{int}[\phi] \equiv g \int d^d x \ \phi^4. \tag{5.22}$$

This is called the **interaction vertex**. We want to establish what the effect of this interaction vertex is on correlations, using as basis the free correlators which we are able to compute:

$$\langle X[\phi] \rangle \simeq \frac{\sum_{n=0}^{\infty} \frac{(-g)^n}{n!} \langle X[\phi] (S_{int}[\phi])^n \rangle_0}{\sum_{n=0}^{\infty} \frac{(-g)^n}{n!} \langle (S_{int}[\phi])^n \rangle_0} \simeq \sum_{n=0}^{n_{max}} X^{(n)} \tag{5.23}$$ CMFT(5.14)

in which $X^{(n)}$ represents the contribution to $\langle X \rangle$ at n-th order in perturbation theory in g.

Let us consider the perturbative expansion of the propagator. Explicitly, we can write

$$\begin{aligned} &\langle \mathcal{G}(\mathbf{x}, \mathbf{x}') \rangle = \langle \phi(\mathbf{x}) \phi(\mathbf{x}') \rangle \\ &= \frac{\langle \phi(\mathbf{x}) \phi(\mathbf{x}') \rangle_0 - g \int d^d y \langle \phi(\mathbf{x}) \phi^4(\mathbf{y}) \phi(\mathbf{x}') \rangle_0 + \frac{g^2}{2} \int d^d y_1 d^d y_2 \langle \phi(\mathbf{x}) \phi(\mathbf{y}_1) \phi^4(\mathbf{y}_2) \phi(\mathbf{x}') \rangle_0 + ...}{1 - g \int d^d y \langle \phi^4(\mathbf{y}) \rangle_0 + \frac{g^2}{2} \int d^d y_1 d^d y_2 \langle \phi^4(\mathbf{y}_1) \phi^4(\mathbf{y}_2) \rangle_0 + ...} \end{aligned} \tag{5.24}$$

Zeroth-order contribution: $\mathcal{G}^{(0)} = \mathcal{G}_0$ is simply the free propagator computed above. First order term:

$$\mathcal{G}^{(1)}(\mathbf{x}, \mathbf{x}') = -g \left(\int d^d y \langle \phi(\mathbf{x}) \phi^4(\mathbf{y}) \phi(\mathbf{x}') \rangle_0 - \langle \phi(\mathbf{x}) \phi(\mathbf{x}') \rangle_0 \int d^d y \langle \phi^4(\mathbf{y}) \rangle_0 \right) \tag{5.25}$$ CMFT(5.15)

The free action is Gaussian, and the average of a product can be calculated using Wick's theorem (3.84. CMFT(3.21) This gives for the first term

$$\begin{aligned} \langle \phi(\mathbf{x}) \phi^4(\mathbf{y}) \phi(\mathbf{x}') \rangle_0 &= 3 \langle \phi(\mathbf{x}) \phi(\mathbf{x}') \rangle_0 [\langle \phi(\mathbf{y}) \phi(\mathbf{y}) \rangle_0]^2 + 12 \langle \phi(\mathbf{x}) \phi(\mathbf{y}) \rangle_0 \langle \phi(\mathbf{y}) \phi(\mathbf{y}) \rangle_0 \langle \phi(\mathbf{y}) \phi(\mathbf{x}') \rangle_0 \\ &= 3 \mathcal{G}_0(\mathbf{x} - \mathbf{x}') \mathcal{G}_0(\mathbf{0})^2 + 12 \mathcal{G}_0(\mathbf{x} - \mathbf{y}) \mathcal{G}_0(\mathbf{0}) \mathcal{G}_0(\mathbf{y} - \mathbf{x}') \end{aligned} \tag{5.26}$$

The total number of terms is $15 = (6-1)!!$ (number of distinct pairings of six objects). For the second term,

$$\langle \phi(\mathbf{x}) \phi(\mathbf{x}') \rangle_0 \langle \phi^4(\mathbf{y}) \rangle_0 = 3 \langle \phi(\mathbf{x}) \phi(\mathbf{x}') \rangle_0 [\langle \phi^2(\mathbf{y}) \rangle_0]^2 = 3 \mathcal{G}_0(\mathbf{x} - \mathbf{x}') \mathcal{G}_0(\mathbf{0})^2. \tag{5.27}$$

Divergences. The factors $\mathcal{G}_0(\mathbf{0})$ contained in the first order terms are disturbing. Written out, these are

$$\mathcal{G}_0(\mathbf{0}) = \int \frac{d^d k}{(2\pi)^d} \frac{1}{k^2 + m^2}. \tag{5.28}$$ CMFT(5.17)

If the dimension $d > 1$, this integral is divergent at large momenta (short wavelengths). This is an **ultraviolet (UV) divergence**. Our theory is meant to be an effective low-energy description, but it is sensitive to high-energy data (for example, an ultraviolet cutoff parameter (*e.g.* a lattice spacing a) used to limit momenta to $k < 1/a$). The proper handling of these effects is the subject of the theory of **renormalization**. Moreover, another problem occurs for dimensions $d \leq 2$: if $m \to 0$, $\mathcal{G}_0(\mathbf{0})$ also diverges because of small momenta, which is a sign of an **infrared (IR) divergence**. How to deal with divergences is a topic for a more advanced course, and we will not cover this here.

Rudiments of diagrammatics. Use a more convenient notation. We represent operator entries as points with a dangling line, and interaction vertices as points with four dangling lines. The field theory average requires us to 'pair up' the fields in order to get a nonzero value. This is represented by joining lines, each different possible joining leading to a different diagram. This is illustrated in Fig. 5.1 for the first-order term for the propagator.

fig:phi4Green1

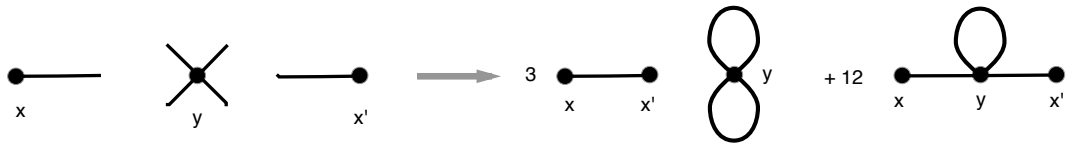

Figure 5.1: First order contribution to the propagator

fig:phi4Green1

We can then do the second-order terms as:

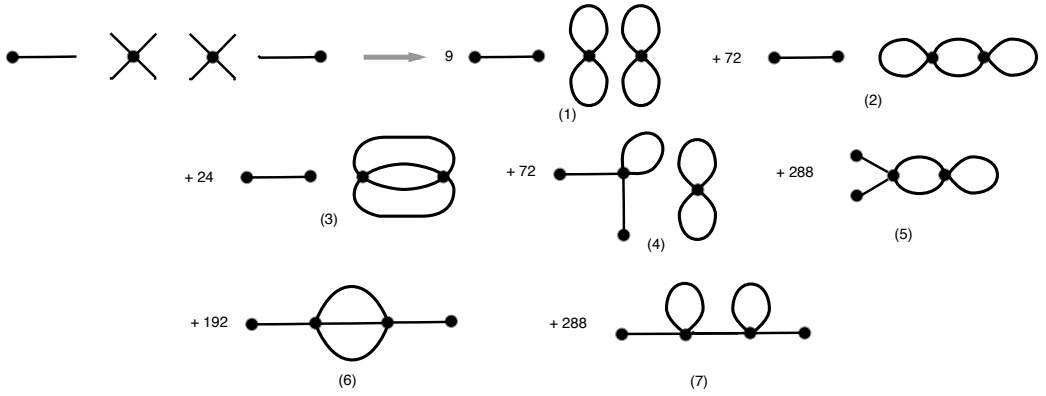

Figure 5.2: Second order contribution to the propagator

fig:phi4Green2

General aspects of diagrammatic approach:

- Efficient representation of the perturbative expansion: at each fixed order in perturbation theory, need to sum over all topologically distinct diagrams.
- No fixed rule as to how to represent a diagram: just don't cut lines. Reshaping, twisting, rotating etc do not change the meaning of a given diagram.
- **connected** diagrams (5,6 and 7 in Fig. 5.2)

fig:phi4Green2

- **one-particle reducible** diagrams (7) (others are one-particle **irreducible**. Generally, diagram whose core region can be cut by severing n lines is **n-particle irreducible** (6: 3-PR).
- the **loop order** of a diagram is the number of closed loops

- There are simple **combinatorics** arguments which fix the 'prefactors' of the diagrams. Here, the prefactor is $n!(4!)^n/S$ where S is the 'symmetry factor' of the diagram (how many permutations we can make between lines in the diagram, without changing it).

- suggestive of **physical interpretation** of the corresponding physical processes (though misleading).

At a given order of perturbation theory, the Green's function obtains contributions from both the numerator and denominator of (5.23). Doing this might sound complicated but in fact it turns out to be *simpler* than the above. The reason is that contributions from the **vacuum graphs** (in which at least one interaction vertex appears which is not connected to any external lines, as (1-4) in Fig. 5.2) all cancel. This is known as the **linked cluster theorem**.

Proof of the linked cluster theorem: Consider a contribution to n-th order to the numerator of (5.23): $\frac{(-g)^n}{n!}\langle X[\phi](\int d^dx\phi^4)^n\rangle_0$. This gives, under contraction, contributions with p-th order vacuum graphs and $n-p$-th order non-vacuum graphs, with p running from 0 to n. The p-th order contribution is

$$\frac{1}{n!}\left(\begin{array}{c} n \\ p \end{array}\right)\langle X[\phi](\int \phi^4)^{n-p}\rangle_0^{n.v}\langle(\int \phi^4)^p\rangle_0 \tag{5.29}$$

with $n.v.$ meaning 'non-vacuum'. Summing over p, the numerator gives

$$\sum_{n=0}^{\infty}\sum_{p=0}^{n}\frac{(-g)^n}{(n-p)!p!}\langle X[\phi](\int \phi^4)^{n-p}\rangle_0^{n.v}\langle(\int \phi^4)^p\rangle_0. \tag{5.30}$$

Rearranging summations, this becomes of factorized form

$$\sum_{n=0}^{\infty}\frac{(-g)^n}{n!}\langle X[\phi](\int \phi^4)^n\rangle_0^{n.v}\sum_{p=0}^{\infty}\frac{(-g)^p}{p!}\langle(\int \phi^4)^p\rangle_0. \tag{5.31}$$

with the p-summation cancelling against the denominator.

To compute the contribution to a given order n in perturbation theory, we thus follow the **Feynman rules**, here for ϕ^4 theory:

- For each operator $\phi(\mathbf{x})$ in X, draw a point (labeled with $\mathbf{x}$) with a dangling line.

- For the n-th order contribution in perturbation theory, draw n vertices with 4 dangling lines, labeling them with coordinates $\mathbf{y}_i$, $i = 1, ..., n$.

- Draw all topologically distinct diagrams obtained by joining the lines pairwise, keeping only connected diagrams.

- Integrate over all vertex coordinates $\mathbf{y}_i$, $i = 1, ..., n$.

- Divide the contribution by the symmetry factor of the diagram.

5.2 Ground state energy of the interacting electron gas

Qualitative aspects When are interactions important ?
Assume each electron occupies a volume r_0^3.
Uncertainty principle: kinetic energy per particle of $\mathcal{O}(\hbar^2/mr_0^2)$.
Interactions: with neighbours, $\mathcal{O}(e^2/r_0)$.
Ratio of scales: **dimensionless density parameter** $\frac{e^2}{r_0}\frac{mr_0^2}{\hbar^2} = \frac{r_0}{a_0} \equiv r_s$ where $a_0 = \frac{\hbar^2}{me^2}$ is the Bohr radius.
The denser the gas, the lower r_s. High density is synonymous with weak interaction effects !!
For $r_s \gg 1$: properties dominated by electron correlations.
At very large r_s, first order transition to **Wigner crystal** is expected.
Most metals: $2 < r_s < 6$, realm of **Landau's Fermi liquid theory**.
Adiabatic continuity: noninteracting GS evolves continuously into interacting GS as strength of the interactions is increased.

5.2.2 Perturbative approach

Free energy:

$$\mathcal{F} = -T \ln \mathcal{Z} \tag{5.32}$$

As coherent state FFI:

$$\mathcal{Z} = \int \mathcal{D}(\bar{\psi}, \psi) e^{-S[\bar{\psi},\psi]}, \tag{5.33}$$

$$S[\bar{\psi},\psi] = \sum_p \bar{\psi}_{p\sigma}(-i\omega_n + \frac{\mathbf{p}^2}{2m} - \mu)\psi_{p\sigma} + \frac{T}{2L^3}\sum_{pp'q} \bar{\psi}_{p+q\sigma}\bar{\psi}_{p'-q\sigma'}V(\mathbf{q})\psi_{p'\sigma'}\psi_{p\sigma} \tag{5.34}$$

where we write from now on $p \equiv (\mathbf{p}, \omega_n)$ as a 'four-momentum'.

Reference scale for correlation energies: free energy of noninteracting gas,

$$\mathcal{F}_0 = -T\sum_{\mathbf{p}\sigma} \ln(1 + e^{-\beta(\frac{\mathbf{p}^2}{2m}-\mu)}) \underset{T\to 0}{\overset{\to}{}} \sum_{\frac{\mathbf{p}^2}{2m}<\mu,\sigma} (\frac{\mathbf{p}^2}{2m} - \mu). \tag{5.35}$$

We have the Fermi momentum $p_F = [2m\mu]^{1/2}$; the volume of the Fermi sphere is $\frac{4}{3}\pi p_F^3$. Each mode occupies a volume $(\frac{2\pi}{L})^3$, so the total number of electrons for a given chemical potential is

$$N(\mu) = 2 \times \frac{L^3}{8\pi^3} \times \frac{4}{3}\pi[2m\mu]^{3/2} = \frac{2^{3/2}}{3}\frac{L^3}{\pi^2}m^{3/2}\mu^{3/2}. \tag{5.36}$$

Energy per particle for the ground state:

$$\frac{E_0(\mu)}{N(\mu)} = \frac{\int_0^{p_F} dpp^2 \frac{p^2}{2m}}{\int_0^{p_F} dpp^2} = \frac{3p_F^2}{10m} = \frac{3}{5}N\mu \tag{5.37}$$

so the average kinetic energy per particle is 3/5 of the Fermi energy. The free energy is

$$\mathcal{F}_0 = E_0 - \mu N = -\frac{2}{5}N\mu \tag{5.38}$$

CMFT(5.19)

(check: using $\frac{\partial N}{\partial \mu} = \frac{3}{2}\frac{N}{\mu}$, we get $-\frac{\partial \mathcal{F}}{\partial \mu} = \frac{2}{5}N - \frac{2}{5}\mu\frac{\partial N}{\partial \mu} = N$ as it should).

Reintroducing interactions. Expanding the interaction term in the partition function yields

$$\mathcal{Z} = \int \mathcal{D}(\bar{\psi},\psi) e^{-S_0[\bar{\psi},\psi]-S_{int}[\bar{\psi},\psi]}$$

$$= \int \mathcal{D}(\bar{\psi},\psi) e^{-S_0[\bar{\psi},\psi]} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(S_{int}[\bar{\psi},\psi]\right)^n$$

$$\rightarrow \mathcal{Z} = \mathcal{Z}_0 \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \langle \left(S_{int}[\bar{\psi},\psi]\right)^n \rangle_0. \tag{5.39}$$

Therefore, the free energy becomes

$$\mathcal{F} = -T \ln \mathcal{Z} = \mathcal{F}_0 - T \ln \left\{ 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \langle \left(S_{int}[\bar{\psi},\psi]\right)^n \rangle_0 \right\}. \tag{5.40}$$

Expanding logs using $\ln(1+x) = \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{m} x^m$ gives

$$\mathcal{F} - \mathcal{F}_0 = -T \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{m} \left\{ \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \langle \left(S_{int}[\bar{\psi},\psi]\right)^n \rangle_0 \right\}^m$$

$$= -T \left\{ \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \langle (S_{int})^n \rangle_0 - \frac{1}{2} \sum_{n_1,n_2=1}^{\infty} \frac{(-1)^{n_1+n_2}}{n_1! n_2!} \langle (S_{int})^{n_1} \rangle_0 \langle (S_{int})^{n_2} \rangle_0 + \frac{1}{3}(3 \text{ summations}) + ... \right\}$$

$$\equiv -T \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \langle (S_{int})^n \rangle_0^c \tag{5.41}$$

where $\langle ... \rangle_0^c$ is the connected part of the average.

To perform the evaluation of the expectation values of the interaction terms, we will use Wick's theorem to rewrite all expectation values as products of single-particle noninteracting Green functions. These are given by

$$\mathcal{G}_0(p) = \langle \bar{\psi}_{p\sigma} \psi_{p\sigma} \rangle = \frac{1}{\mathcal{Z}_0} \int \mathcal{D}(\bar{\psi},\psi) e^{-S_0[\bar{\psi},\psi]} \bar{\psi}_{p\sigma} \psi_{p\sigma}. \tag{5.42}$$

Writing the numerator and denominator explicitly as a product of decoupled Grassmann integrals, the only term that does not cancel is the one for p, σ, so

$$\mathcal{G}_0(p) = \frac{\int d(\bar{\psi}_{p\sigma}, \psi_{p\sigma}) e^{-\bar{\psi}_{p\sigma}[-i\omega_n + \frac{\mathbf{p}^2}{2m} - \mu]\psi_{p\sigma}} \bar{\psi}_{p\sigma} \psi_{p\sigma}}{\int d(\bar{\psi}_{p\sigma}, \psi_{p\sigma}) e^{-\bar{\psi}_{p\sigma}[-i\omega_n + \frac{\mathbf{p}^2}{2m} - \mu]\psi_{p\sigma}}} = \frac{1}{i\omega_n + \mu - \frac{\mathbf{p}^2}{2m}} = \mathcal{G}_0(p)$$

Diagrammatic perturbation theory: **Feynman rules**

• Coulomb interaction: wavy line, argument **q**

• Contraction $\langle \bar{\psi}_{p\sigma} \psi_{p\sigma} \rangle_0$: free Green's function $\mathcal{G}_0(p)$ written as a line with arrow following the flow of charge, four-momentum and spin as arguments

• all momenta conserved at vertices

• fermion loop: extra factor of (-1)

• don't forget sum over spins !

First order correction to $\mathcal{F}$

$$\mathcal{F}^{(1)} = \frac{T^2}{2L^3} \sum_{pp'q} \sum_{\sigma\sigma'} \langle \bar{\psi}_{p+q\sigma} \bar{\psi}_{p'-q\sigma'} V(\mathbf{q}) \psi_{p'\sigma'} \psi_{p\sigma} \rangle_0 \tag{5.43}$$

Basic interaction vertex:

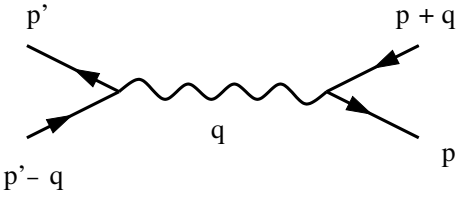

Figure 5.3: Basic interaction vertex

fig:F1_vertex

Two possible contractions: $(1,4)(2,3)$ and $(1,3)(2,4)$.

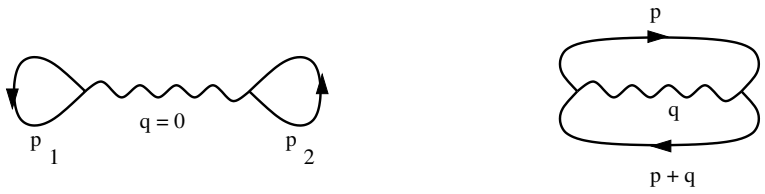

Figure 5.4: Hartree (left) and Fock (right) contributions to the first-order free energy correction.

fig:F1_Hartre

1) Hartree contribution:

$$(-1)^2 \frac{T^2}{2L^3} \times 4 \times (\sum_p \langle \bar{\psi}_{p\sigma} \psi_{p\sigma} \rangle_0)^2 V(\mathbf{q}=0) \tag{5.44}$$

This interaction is a 'classical'-like charge coupling. We usually take this to vanish since the zero-momentum Coulomb potential vanishes by charge neutrality.

2) Fock contribution:

$$-\frac{T^2}{2L^3} \sum_{p,q} \sum_{\sigma} V(\mathbf{q}) \langle \bar{\psi}_{p+q\sigma} \psi_{p+q\sigma} \rangle_0 \langle \bar{\psi}_{p\sigma} \psi_{p\sigma} \rangle_0 = -\frac{T^2}{L^3} \sum_{p,p'} \mathcal{G}_0(p) \mathcal{G}_0(p') V(\mathbf{p}'-\mathbf{p}) \tag{5.45}$$

CMFT(5.23a)

We can use (4.75) to do summations over the two Matsubara frequencies:

CMFT(4.39)

$$... = \frac{-1}{L^3} \sum_{\mathbf{p},\mathbf{p}'} n_F(\varepsilon_{\mathbf{p}}) n_F(\varepsilon_{\mathbf{p}'}) \frac{e^2}{|\mathbf{p}-\mathbf{p}'|^2} \;\; \overset{\rightarrow}{T \to 0} \;\; \frac{-1}{L^3} \sum_{\varepsilon_{\mathbf{p}}, \varepsilon_{\mathbf{p}'} < \mu} \frac{e^2}{|\mathbf{p}-\mathbf{p}'|^2} \tag{5.46}$$

This last integration (over two Fermi surfaces) can be done. Base spherical coordinates for $\mathbf{p}'$ on $\mathbf{p}$ vector. Then, $p_z - p'_z = p - p'\cos\theta$, $p_x - p'_x = -p'\sin\theta\sin\phi$, $p_y - p'_y = -p\sin\theta\cos\phi$ and $|\mathbf{p}-\mathbf{p}'|^2 = (p-p'\cos\theta)^2 + p'^2\sin^2\theta = p^2 + p'^2 - 2pp'\cos\theta$. The integral becomes

$$\begin{aligned}
&\frac{-1}{L^3}\left(\frac{L^3}{(2\pi)^3}\right)^2 4\pi\int_0^{p_F} dpp^2\int_0^{p_F} dp'p'^2\int_0^{\pi} d\theta\frac{2\pi p'^2\sin\theta}{p^2+p'^2-2pp'\cos\theta}\\
&\qquad = \frac{-L^3 4}{2^6\pi^4}\int_0^{p_F} dpp\int_0^{p_F} dp'p'\int_0^{\pi} d\theta\frac{d}{d\theta}\ln[p^2+p'^2-2pp'\cos\theta]\\
&= \frac{-L^3}{16\pi^4}\int_0^{p_F} dpp\int_0^{p_F} dp'p'\ln\frac{(p+p')^2}{(p-p')^2} = \frac{-L^3}{4\pi^4}\int_0^{p_F} dpp\int_0^{p} dp'p'\ln\frac{p+p'}{p-p'} \qquad (5.47)
\end{aligned}$$

Using $\int_0^1 dxx\ln\frac{1+x}{1-x} = \left[\frac{x^2-1}{2}\ln\frac{1+x}{1-x} + x\right]|_0^1 = 1$ finally yields

$$\mathcal{F}^{(1)}_{\text{Fock}} = -\frac{L^3}{16\pi^4}p_F^4. \qquad (5.48)$$

CMFT(5.23b)

Second order correction to $\mathcal{F}$

$$\mathcal{F}^{(2)} = -\frac{T}{2}\left(\frac{T}{2L^3}\right)^2 \left\langle \left(\sum_{pp'q} \sum_{\sigma\sigma'} \bar{\psi}_{p+q\sigma} \bar{\psi}_{p'-q\sigma'} V(\mathbf{q}) \psi_{p'\sigma'} \psi_{p\sigma} \right)^2 \right\rangle_0^c \tag{5.49}$$

Basic vertices:

Number of possible contractions: 4! = 24. 4 with 0 interconnections, 16 with 2 interconnections, and 4 with 4 interconnections.

Draw the 24 Feynman diagrams

Putting things together, we have three types of nonzero contributions:

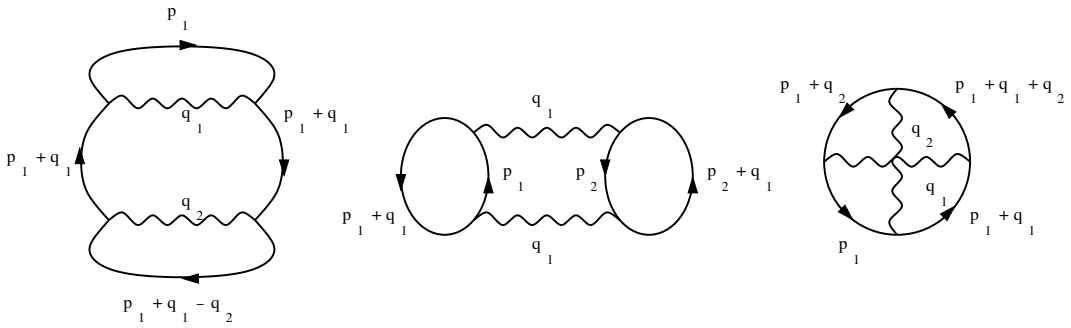

Figure 5.5: The three types of contributions to the second-order correction to the free energy.

fig:F2_3types

a) 4 times ...

Contribution:

$$\begin{aligned} 4 \times \frac{-T}{2}\left(\frac{T}{2L^3}\right)^2 \times 2 \times (-1) \sum_{p_1 q_1 q_2} \mathcal{G}_0(p_1)\mathcal{G}_0^2(p_1+q_1)\mathcal{G}_0(p_1+q_1-q_2)V(\mathbf{q}_1)V(\mathbf{q}_2) \\ = \frac{T^3}{L^6} \sum_{p_1 q_1 q_2} \mathcal{G}_0(p_1)\mathcal{G}_0^2(p_1+q_1)\mathcal{G}_0(p_1+q_1-q_2)V(\mathbf{q}_1)V(\mathbf{q}_2) \end{aligned} \tag{5.50}$$

b) 2 times ... Contribution:

$$\begin{aligned} 2 \times \frac{-T}{2}\left(\frac{T}{2L^3}\right)^2 \times 4 \times (-1)^2 \sum_{p_1 p_2 q_1} \mathcal{G}_0(p_1)\mathcal{G}_0(p_1+q_1)\mathcal{G}_0(p_2)\mathcal{G}_0(p_2+q_1)V^2(\mathbf{q}_1) \\ = -\frac{T^3}{L^6} \sum_{p_1 p_2 q_1} \mathcal{G}_0(p_1)\mathcal{G}_0(p_1+q_1)\mathcal{G}_0(p_2)\mathcal{G}_0(p_2+q_1)V^2(\mathbf{q}_1) \end{aligned} \tag{5.51}$$

c) 2 times ... Contribution:

$$2 \times \frac{-T}{2}\left(\frac{T}{2L^3}\right)^2 \times 2 \times (-1) \sum_{p_1 q_1 q_2} \mathcal{G}_0(p_1)\mathcal{G}_0(p_1+q_1)\mathcal{G}_0(p_1+q_2)\mathcal{G}_0(p_1+q_1+q_2)V(\mathbf{q}_1)V(\mathbf{q}_2)$$
$$= \frac{T^3}{2L^6} \sum_{p_1 q_1 q_2} \mathcal{G}_0(p_1)\mathcal{G}_0(p_1+q_1)\mathcal{G}_0(p_1+q_2)\mathcal{G}_0(p_1+q_1+q_2)V(\mathbf{q}_1)V(\mathbf{q}_2) \quad (5.52)$$

The b) part has a double integration p_1, p_2 that is unconstrained (2 fermion loops). This contribution dominates, having a higher power of system size.

Higher orders in perturbation theory The idea that diagrams with more fermion loops (at a given order of PT) are dominant generalizes to higher order.

At order n, the dominant graph is the 'ring graph'

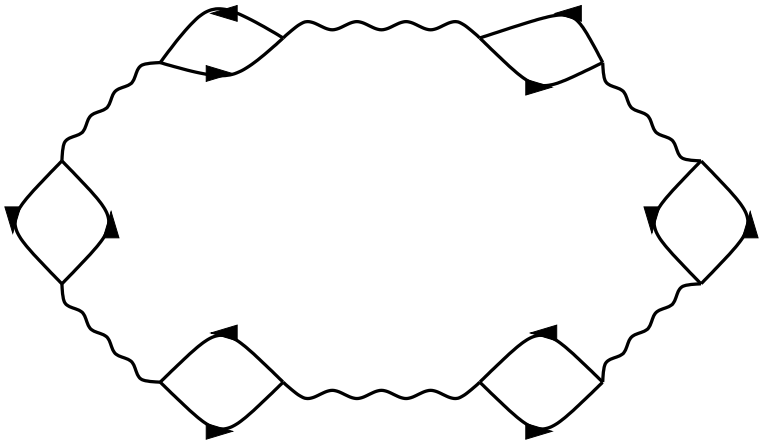

Figure 5.6: The ring graph for the RPA approximation to the free energy.

fig:RPA_F

This contributes the **random phase approximation** term to the free energy,

$$\mathcal{F}^{(n)}_{RPA} = -\frac{T}{2n}\sum_q \left(\frac{2T}{L^3}V(\mathbf{q})\sum_p \mathcal{G}_0(p)\mathcal{G}_0(p+q)\right)^n \quad (5.53)$$ CMFT(5.26)

(prefactor: $(n-1)!/n!$, since there are $(n-1)!$ distinct ways of arranging loops on a ring; alternately, symmetry factor of n from rotation symmetry). Summing over n yields

$$\mathcal{F}_{RPA} = \frac{T}{2}\sum_q \ln\left[1 - V(\mathbf{q})\Pi(q)\right] \quad (5.54)$$ CMFT(5.27)

where the **polarization operator** is defined as

$$\Pi(q) \equiv \frac{2T}{L^3}\sum_p \mathcal{G}_0(p)\mathcal{G}_0(p+q) = \Pi(-q) \quad (5.55)$$ CMFT(5.28)

From results of problem 4.5.5, we can write

$$\Pi_{\mathbf{q},\omega_n} = \frac{2T}{L^3}\sum_p \frac{1}{i\omega_n - \xi_{\mathbf{p}}}\frac{1}{i\omega_{n+m} - \xi_{\mathbf{p+q}}} = \frac{2}{L^3}\sum_{\mathbf{p}} \frac{n_F(\varepsilon_{\mathbf{p+q}}) - n_F(\varepsilon_{\mathbf{p}})}{i\omega_n + \xi_{\mathbf{p+q}} - \xi_{\mathbf{p}}} \tag{5.56}$$ CMFT(5.29)

Sum over momentum yields (see Info block on p. 220)

$$\Pi_{\mathbf{q},\omega_n} = -\nu_0\left[1 - \frac{i\omega_n}{v_F q}\ln\frac{i\omega_n + v_F q}{i\omega_n - v_F q}\right] \tag{5.57}$$ CMFT(5.30)

where ν_0 is the density of states per unit volume at the Fermi surface,

$$\nu_0 \equiv \frac{1}{L^d}\sum_{\mathbf{p},\sigma}\delta(\varepsilon_{\mathbf{p}} - \mu) = 2\int\frac{d^3p}{(2\pi)^3}\delta(\varepsilon_{\mathbf{p}} - \mu) = \frac{mp_F}{\pi^2} \tag{5.58}$$ CMFT(5.31)

since $\frac{2\times 4\pi}{8\pi^3}\int_0^{p_F} dpp^2\delta(\frac{p^2}{2m} - \mu) = \frac{mp_F}{\pi^2}$.

Conceptual meaning of RPA and connection to screening. Compute expectation value of number operator $N = -\partial_\mu \mathcal{F}$. Compare first-order result $N^{(1)} = -\partial_\mu \mathcal{F}^{(1)}$ with RPA result $N_{RPA} = -\partial_\mu \mathcal{F}_{RPA}$. We have from (CMFT(5.23a) 5.45)

$$N^{(1)} = \frac{T^2}{L^3}\sum_{p,p'}\partial_\mu\left[\mathcal{G}_0(p)\mathcal{G}_0(p')\right]V(\mathbf{p}' - \mathbf{p}) \tag{5.59}$$

First order: use $\partial_\mu \mathcal{G}_0(p) = -\mathcal{G}_0^2(p)$ so

$$N^{(1)} = -\frac{2}{T^2}L^3\sum_{pq}\mathcal{G}_0^2(p)\mathcal{G}_0(p+q)V(\mathbf{q}). \tag{5.60}$$

Diagram:

Draw diagram

RPA: from (CMFT(5.27) 5.54),

$$N_{RPA} = \frac{T}{2}\sum_q \frac{V(\mathbf{q})\partial_\mu\Pi(q)}{1 - V(\mathbf{q})\Pi(q)}. \tag{5.61}$$

But we have

$$\partial_\mu\Pi(q) = -\frac{2T}{L^3}\sum_p\left(\mathcal{G}_0^2(p)\mathcal{G}_0(p+q) + \mathcal{G}_0(p)\mathcal{G}_0^2(p+q)\right) \tag{5.62}$$

so we get

$$N_{RPA} = -\frac{2T^2}{L^3}\sum_q\frac{V(\mathbf{q})}{1 - V(\mathbf{q})\Pi(q)}\sum_p\mathcal{G}_0^2(p)\mathcal{G}_0(p+q) = -\frac{2T^2}{L^3}\sum_q V_{eff}(\mathbf{q})\sum_p\mathcal{G}_0^2(p)\mathcal{G}_0(p+q) \tag{5.63}$$

where

$$V_{eff}(\mathbf{q}) \equiv \frac{1}{V(\mathbf{q})^{-1} - \Pi(q)} \equiv \frac{V(\mathbf{q})}{\epsilon(q)} \tag{5.64}$$

defines the **dielectric function** $\epsilon(q) \equiv 1 - V(\mathbf{q})\Pi(q)$.

So: RPA like first order, but with 'bare' Coulomb replaced by effective interaction summing over polarization bubbles.

Diagrammatics of polarization bubbles

$$V_{eff} = V + V\pi V_{eff} \rightarrow V_{eff} = \frac{V}{1 - V\Pi} \tag{5.65}$$

Connection with electromagnetic response: electric displacement field given by product of dielectric function with electric field in medium,

$$\mathbf{D}(\mathbf{q}, \omega) = \epsilon(\mathbf{q}, \omega)\mathbf{E}(\mathbf{q}, \omega) \tag{5.66}$$

with

$$\epsilon(\mathbf{q}, \omega) = 1 + 4\pi\chi(\mathbf{q}, \omega) \tag{5.67}$$

where χ is the electromagnetic susceptibility.

Identifying $\mathbf{E}$ with gradient of dressed potential V_{eff}, $\mathbf{D}$ with gradient of bare potential V,

$$4\pi\chi(\mathbf{q}, \omega) = -V(\mathbf{q})\Pi(\mathbf{q}, \omega) \tag{5.68}$$

so susceptibility is proportional to polarization operator[CMFT(5.30)]

Simplification in limiting cases: Lindhard function (5.57) depends on dimensionless ratio of two characteristic length scales:

'wavelength' q^{-1} and distance v_F/ω traveled by excitations at Fermi velocity in characteristic time ω^{-1}.

For low frequencies: $v_F/\omega \gg q^{-1}$: gas has enough time to screen out fluctuations, **static limit**. Expand:

$$\begin{aligned} \Pi(\mathbf{q}, \omega_n) &\simeq_{\omega \ll q v_F} -\nu_0 + \mathcal{O}(\omega/v_F q), \\ V_{eff}(q) \simeq_{\omega \ll q v_F} \frac{1}{V(\mathbf{q})^{-1} + \nu_0} &= \frac{4\pi e^2}{q^2 + 4\pi e^2 \nu_0} = \frac{4\pi e^2}{q^2 + \lambda^{-2}} \end{aligned} \tag{5.69}$$

where $\lambda \equiv (4\pi e^2 \nu_0)^{-1/2}$ is the **Thomas-Fermi screening length**. Inverse FT:

$$V_{eff}(\mathbf{r}) = e^2 \frac{e^{-|\mathbf{r}|/\lambda}}{|\mathbf{r}|} \tag{5.70}$$

so potential is screened on length scale $\sim \lambda$.

Chapter 6

Effective theories

ET

6. Broken symmetry and collective phenomena

6.1 Mean field theory

Let us imagine a very simple situation in which we have some basic theory

$$H = H_0 + H_{int} \tag{6.1}$$

with H_0 being a simple one-body Hamiltonian, and the interaction term being a product of two one-body operators

$$H_{int} = \mathcal{O}_1 \mathcal{O}_2. \tag{6.2}$$

Let us imagine that the operators $\mathcal{O}_i$ are such that they mildly fluctuate around some 'mean field' value,

$$\mathcal{O}_i = \langle \mathcal{O}_i \rangle_{MF} + (\mathcal{O}_i - \langle \mathcal{O}_i \rangle_{MF}) \equiv \langle \mathcal{O}_i \rangle_{MF} + \delta \mathcal{O}_i. \tag{6.3}$$

We can then rewrite the interaction term as

$$H_{int} = \langle \mathcal{O}_1 \rangle_{MF} \langle \mathcal{O}_2 \rangle_{MF} + \langle \mathcal{O}_1 \rangle_{MF} \delta \mathcal{O}_2 + \delta \mathcal{O}_1 \langle \mathcal{O}_2 \rangle_{MF} + \delta \mathcal{O}_1 \delta \mathcal{O}_2. \tag{6.4}$$

If the fluctuations of $\mathcal{O}_i$ are small, we can neglect the last term (quadratic in fluctuations) and keep only the first two terms, that is keep only up to linear terms in the fluctuations. Since the effective Hamiltonian

$$H_{eff} = H_0 + \langle \mathcal{O}_1 \rangle_{MF} \mathcal{O}_2 + \mathcal{O}_1 \langle \mathcal{O}_2 \rangle_{MF} - \langle \mathcal{O}_1 \rangle_{MF} \langle \mathcal{O}_2 \rangle_{MF} \tag{6.5}$$

then contains only single-body terms (in which $\langle \mathcal{O}_i \rangle_{MF}$ are now parameters), it can usually be solved exactly. This allows to calculate (among others) the averages

$$\langle \mathcal{O}_i \rangle_{eff} = \frac{1}{\mathcal{Z}_{eff}} \text{ Tr } \mathcal{O}_i e^{-\beta H_{eff}}. \tag{6.6}$$

One must then ensure *self-consistency* of the theory by requiring

$$\langle \mathcal{O}_i \rangle_{eff} = \langle \mathcal{O}_i \rangle_{MF}, \tag{6.7}$$

in other words that the prediction from the effective theory are consistent with the assumptions; these self-consistency conditions are usually sufficient to determine all parameters $\langle \mathcal{O}_i \rangle_{MF}$.

This is the essence of **mean field theory**, in which fluctuations are coupled only to non-fluctuating averages.

Mean field theory is somewhat of an art, in the sense that typical problems can be 'decomposed' in different ways, each leading to their own mean-field solution. Which is best, and whether the construction makes any sense, depends individually on each problem.

Generically, we would like to decompose two-body terms (which can't be handled exactly) into single-body terms (which can be). Let us imagine that we have four operators,

$$a_1^\dagger a_2^\dagger a_3 a_4 \tag{6.8}$$

which we would like to write in mean field. If these were free particles, taking an expectation value over a number-preserving theory would yield (using Wick's theorem)

$$\langle a_1^\dagger a_2^\dagger a_3 a_4 \rangle = \langle a_1^\dagger a_4 \rangle \langle a_2^\dagger a_3 \rangle + \zeta \langle a_1^\dagger a_3 \rangle \langle a_2^\dagger a_4 \rangle. \tag{6.9}$$

For example, a (particle-number preserving) decoupling which is consistent with this is given by

$$\begin{aligned} a_1^\dagger a_2^\dagger a_3 a_4 \simeq a_1^\dagger a_4 \langle a_2^\dagger a_3 \rangle_{MF} + a_2^\dagger a_3 \langle a_1^\dagger a_4 \rangle_{MF} + \zeta a_1^\dagger a_3 \langle a_2^\dagger a_4 \rangle_{MF} + \zeta a_2^\dagger a_4 \langle a_1^\dagger a_3 \rangle_{MF} + \\ - \langle a_1^\dagger a_4 \rangle_{MF} \langle a_2^\dagger a_3 \rangle_{MF} - \zeta \langle a_1^\dagger a_3 \rangle_{MF} \langle a_2^\dagger a_4 \rangle_{MF} \end{aligned} \tag{6.10}$$

6.2 Plasma theory of the interacting electron gas

$$S[\bar{\psi},\psi] = \sum_p \bar{\psi}_{p\sigma}(-i\omega_n + \frac{\mathbf{p}^2}{2m} - \mu)\psi_{p\sigma} + \frac{T}{2L^3}\sum_{pp'q}\bar{\psi}_{p+q\sigma}\bar{\psi}_{p'-q\sigma'}V(\mathbf{q})\psi_{p'\sigma'}\psi_{p\sigma} \tag{6.11}$$

with $V(\mathbf{q}) = \frac{4\pi e^2}{|\mathbf{q}|^2}$. Not quadratic, quartic ! No exact calculation. But: good trick: decouple the interaction by introducing auxiliary field. Look at interaction term in action:

$$e^{-S_{int}} = \exp\left(-\frac{T}{2L^3}\sum_q V(\mathbf{q})\rho_q\rho_{-q}\right), \qquad \rho_q \equiv \sum_{p\sigma}\bar{\psi}_{p+q\sigma}\psi_{p\sigma}. \tag{6.12}$$

Consider a simple Gaussian integral over an auxiliary bosonic field variable ϕ:

$$\int \mathcal{D}\phi \exp\left(-\frac{e^2\beta}{2L^3}\sum_q \phi_q V^{-1}(\mathbf{q})\phi_{-q}\right) \equiv 1 \tag{6.13}$$

(which defines the measure $\mathcal{D}\phi$). Shifting $\phi_q \to \phi_q - \frac{i}{e\beta}V(\mathbf{q})\rho_q$, get

$$1 = \int \mathcal{D}\phi \exp\left(-\frac{e^2\beta}{2L^3}\sum_q \phi_q V^{-1}(\mathbf{q})\phi_{-q} + \frac{ie}{2L^3}\sum_q(\phi_q\rho_{-q} + \phi_{-q}\rho_q) + \frac{1}{2\beta L^3}\sum_q \rho_q V(\mathbf{q})\rho_{-q}\right) \tag{6.14}$$

where the last factor is independent of ϕ. Therefore, we have the identity

$$e^{-S_{int}} = \int \mathcal{D}\phi \exp\left(-\frac{e^2\beta}{2L^3}\sum_q \phi_q V^{-1}(\mathbf{q})\phi_{-q} + \frac{ie}{L^3}\sum_q \phi_q\rho_{-q}\right). \tag{6.15}$$

This is a simple example of a **Hubbard-Stratonovich transformation**: decoupling of interaction at the expense of introducing an additional field.

The partition function then becomes

$$\mathcal{Z} = \int \mathcal{D}\phi \int \mathcal{D}(\bar{\psi},\psi)e^{-S[\phi,\bar{\psi},\psi]}, \tag{6.16}$$

with the effective action

$$S[\phi,\bar{\psi},\psi] = \frac{\beta}{8\pi L^3}\sum_q \phi_q\mathbf{q}^2\phi_{-q} + \sum_{pp'\sigma}\bar{\psi}_{p\sigma}\left[\left(-i\omega_n + \frac{\mathbf{p}^2}{2m} - \mu\right)\delta_{pp'} + \frac{ie}{L^3}\phi_{p'-p}\right]\psi_{p'\sigma} \tag{6.17}$$

CMFT(6.1)

Performing the fermionic integration yields

$$\mathcal{Z} = \int \mathcal{D}\phi \exp\left(-\frac{\beta}{8\pi L^3}\sum_q \phi_q\mathbf{q}^2\phi_{-q}\right) \det\left[-i\hat{\omega} + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + \frac{ie}{L^3}\hat{\phi}\right]. \tag{6.18}$$

Use now the identity $\ln \det \hat{A} = \mathrm{Tr}\ln\hat{A}$, the partition function is finally written as

$$\mathcal{Z} = \int \mathcal{D}\phi e^{-S[\phi]}, \tag{6.19}$$

with effective action

$$S[\phi] = \frac{\beta}{8\pi L^3}\sum_q \phi_q\mathbf{q}^2\phi_{-q} - \mathrm{Tr}\ln\left[-i\hat{\omega} + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + \frac{ie}{L^3}\hat{\phi}\right]. \tag{6.20}$$

CMFT(6.4)

Mean field theory: stationary phase analysis.

$$\frac{\delta S[\phi]}{\delta \phi_q} = 0, \forall q(\mathbf{q} \neq 0, \omega) \tag{6.21}$$

we have (using $\mathcal{G}^{-1} = -i\hat{\omega} + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + \frac{ie}{L^3}\hat{\phi}$)

$$\begin{aligned} \frac{\delta}{\delta \phi_q} \text{ Tr} \ln \mathcal{G}^{-1} = & \text{ Tr}\left(\hat{\mathcal{G}} \frac{\delta}{\delta \phi_q} \hat{\mathcal{G}}^{-1}\right) \\ = 2 \sum_{q_1 q_2} \hat{\mathcal{G}}_{q_1 q_2} \left(\frac{\delta}{\delta \phi_q} \hat{\mathcal{G}}^{-1}\right)_{q_2 q_1} = & \frac{2ie}{L^3} \sum_{q_1 q_2} \hat{\mathcal{G}}_{q_1 q_2} \delta_{q_1 - q_2, q} \end{aligned} \tag{6.22}$$

so saddle-point condition is (using $\left(\frac{\delta}{\delta \phi_q}\hat{\phi}\right)_{q_1 q_2} = \delta_{q_1 - q_2, q}$)

$$\frac{\delta}{\delta \phi_q} S[\phi] = \frac{\beta}{4\pi L^3} \mathbf{q}^2 \phi_{-q} - \frac{2ie}{L^3} \sum_{q_1} \mathcal{G}_{q_1, q_1 - q} = 0. \tag{6.23}$$ CMFT(6.5)

Solution: guess that $\phi_{\mathbf{q},\omega} = 0$ if either $\mathbf{q}$ or ω is $\neq 0$. Then, Green function is diagonal, $\mathcal{G}_{q_1 q_2} \propto \delta_{q_1, q_2}$, for $q \neq 0$ both terms in (6.23) vanish. Moreover, identify $\hat{\phi} = 0$ as solution because of charge neutrality (which requires $\phi_{q=0} = 0$, which comes from $V(\mathbf{q})$ vanishing for $\mathbf{q} = 0$).

Expanding the functional in fluctuations around $\phi = 0$:

$$\text{Tr } \ln \hat{\mathcal{G}}^{-1} = \text{ Tr } \ln \hat{\mathcal{G}}_0^{-1} + \frac{ie}{L^3} \text{ Tr } (\hat{\mathcal{G}}_0 \hat{\phi}) + \frac{1}{2} (\frac{e}{L^3})^2 \text{ Tr } (\hat{\mathcal{G}}_0 \hat{\phi} \hat{\mathcal{G}}_0 \hat{\phi}) + ... \tag{6.24}$$

where $\hat{\mathcal{G}}_0^{-1} \equiv -i\hat{\omega} + \frac{\hat{\mathbf{p}}^2}{2m} - \mu$. Second order term:

$$(\frac{e}{L^3})^2 \sum_{pq} \mathcal{G}_{0,p} \phi_q \mathcal{G}_{0,p-q} \phi_{-q} = \frac{e^2}{2TL^3} \sum_q \Pi_q \phi_q \phi_{-q} \tag{6.25}$$

where $\Pi(q)$ is the polarization operator (5.55). Therefore, the effective action becomes (linear term vanishes) CMFT(5.28)

$$S_{eff}[\phi] = \frac{1}{2TL^3} \sum_q \phi_q \left(\frac{\mathbf{q}^2}{4\pi} - e^2 \Pi_q\right) \phi_{-q} + \mathcal{O}(\phi^4) \tag{6.26}$$ CMFT(6.6)

so the partition function is

$$\mathcal{Z}_{eff} = \mathcal{Z}_0 \prod_q \left(1 - \frac{4\pi e^2}{q^2} \Pi_q\right)^{-1/2} \tag{6.27}$$

and the free energy becomes

$$\mathcal{F}_{eff} = -T \ln \mathcal{Z}_{eff} = \mathcal{F}_0 + \frac{T}{2} \sum_q \ln \left(1 - \frac{4\pi e^2}{q^4} \Pi_q\right) \tag{6.28}$$

which is exactly $\mathcal{F}_{RPA}$ from (5.54). CMFT(5.27)

Summary: diagrammatics versus field integration.

Diagrammatics: sum up Feynman diagrams
- 'brute force'
- combinatorics
- messy, no clear physical picture.

Field integration: decouple, seek saddle pt, expand around it
- well-defined, 'automated', flexible program
- no mess with diagrams, less risk of missing important contributions
- most important: extensibility

6.3 Bose-Einstein condensation and superfluidity

Weakly interacting Bose gas:

$$S[\bar{\psi},\psi] = \int d^d r \int d\tau \left[\bar{\psi}(\mathbf{r},\tau)(\partial_\tau + \hat{H}_0 - \mu)\psi(\mathbf{r},\tau) + \frac{g}{2}(\bar{\psi}(\mathbf{r},\tau)\psi(\mathbf{r},\tau))^2\right] \tag{6.29}$$ CMFT(6.7)

6.3.1 Bose-Einstein condensation

Possibility: at low T, the GS of a bosonic system can involve the condensation of a finite fraction of all the particles into a single state (Einstein, 1925). Simplest case: noninteracting gas, basis in which the one-particle Hamiltonian is diagonal. We then have

$$\mathcal{Z}_0 \equiv \mathcal{Z}|_{g=0} = \int \mathcal{D}(\bar{\psi},\psi) \exp\left[-\sum_{an} \bar{\psi}_{an}(-i\omega_n + \varepsilon_a - \mu)\psi_{an}\right]. \tag{6.30}$$ CMFT(6.7a)

Assume that $\varepsilon_a \geq 0$ with ground state $\varepsilon_0 = 0$. To ensure stability, the chemical potential must be negative (otherwise $\varepsilon_a - \mu$ could change sign for low-lying states).

Number of particles: given by

$$N(\mu) = T\sum_{na} \frac{1}{i\omega_n - \varepsilon_a + \mu} = \sum_a n_B(\varepsilon_a) \tag{6.31}$$ CMFT(6.7b)

with $n_B(\varepsilon) = 1/(e^{\beta(\varepsilon-\mu)} - 1)$. For a given number N of particles, this determines $\mu(T)$. As T goes down, so does $n_B(\varepsilon_{a\neq 0})$, and thus $\mu(T)$ has to increase with decreasing temperature, to preserve the total particle number.

Below a certain T_c, the maximum value of $\mu = 0$ is not enough to keep $n_B(\varepsilon_{a\neq 0})$ large enough, and we get

$$\sum_{a>0} n_B(\varepsilon_a)|_{\mu=0} \equiv_{T<T_c} N_1 < N, \tag{6.32}$$

meaning that below this temperature, the number of particles in the lowest state, N_0 becomes macroscopic, with $N_0 + N_1 = N$.

Exercise: for a 3D system of free particles, $\varepsilon_k = \hbar^2 k^2/2m$, show that $T_c = c_0\hbar^2/ma^2$ where $a = \rho^{-1/3}$ is the average interparticle spacing ($\rho = N/V$ is the density), and c_0 is a constant of order unity. Show that for $T < T_c$, the density of particles in the condensate ($\mathbf{k} = 0$) is $\rho_0(T) = \rho[1 - (T/T_c)^{3/2}]$.

In terms of field operators, we will want to keep the zero energy state counted separately. In the action, the ψ_0 mode corresponds then to a Lagrange multiplier fixing the number of particles. The (reduced) action takes the form

$$S_0[\bar{\psi},\psi] = -\bar{\psi}_0\beta\mu\psi_0 + \sum_{a\neq 0,n} \bar{\psi}_{an}(-i\omega_n + \varepsilon_a - \mu)\psi_{an}, \tag{6.33}$$

where (for the purpose of calculations) μ is kept different from zero. This allows for example to write the particle number condition,

$$N = -\partial_\mu F_0|_{\mu=0} = T\partial_\mu \ln \mathcal{Z}_0|_{\mu=0} = \bar{\psi}_0\psi_0 + T\sum_{a\neq 0,n} \frac{1}{i\omega_n - \varepsilon_a} = \bar{\psi}_0\psi_0 + N_1 \tag{6.34}$$ CMFT(6.8)

now and further on.

The weakly interacting Bose gas

We now reintroduce the interaction coupling. Dominant contribution to the action at low temperature:

$$TS[\bar{\psi}_0, \psi_0] = -\mu\bar{\psi}_0\psi_0 + \frac{g}{2L^d}(\bar{\psi}_0\psi_0)^2. \tag{6.35}$$

CMFT(6.9)

The stability of the action is now guaranteed by the interaction, no matter how small $g > 0$ is.

Saddle-point analysis: varying (6.35) w.r. to ψ_0 yields

$$\psi_0(-\mu + \frac{g}{L^2}\bar{\psi}_0\psi_0) = 0, \tag{6.36}$$

which is solved by any field such that $|\psi_0| = \sqrt{\mu L^d/g} \equiv \gamma$. Remarks: 1) for $\mu < 0$, no stable condensate exists ($\psi_0 = 0$). 2) below the condensation threshold (so for $\mu \geq 0$), any ψ_0 s.t. $|\psi_0| = \sqrt{\mu L^d/g}$ solves the saddle-point equation (note: $\bar{\psi}_0\psi_0 \sim L^d$, so the ground state is macroscopically occupied). 3) the phase of ψ_0 is a free variable: any $\psi_0 = \gamma\exp(i\phi)$ with $\phi \in [0, 2\pi]$ solves the saddle-point equation.

6.4 Superconductivity

First observed by H. Kammerlingh Onnes in 1911 in Leiden.

Two aspects: 1) drop of electrical resistivity to zero below critical temperature. 2) perfect diamagnetism: a SC expels all magnetic flux from its interior.

6.4.1 Basic concepts of BCS theory

Time scales for electrons: $\sim \varepsilon_F^{-1}$. For ions: $\sim \omega_D^{-1}$ (inverse of Debye frequency). But $\omega_D^{-1} \gg \varepsilon_F^{-1}$ so ...

Attractive interaction leads to bound states of pairs of electrons, **Cooper pairs**, which mimic bosonic particles.

Figure on p. 273: shell of thickness ω_D/v_F around Fermi surface; large phase space for scattering of pairs. Weak interaction but large phase space: possibly important effect !!

Simplified model: the **BCS Hamiltonian**

$$\hat{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma} - \frac{g}{L^d} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'+\mathbf{q}\downarrow} c_{\mathbf{k}'\uparrow} \tag{6.37}$$

CMFT(6.14)

6.4.3 Mean-field theory of superconductivity

Due to the pairing interaction, the system develops an instability towards the formation of Cooper pairs.

Assume that the ground state $|\Omega_s\rangle$ of the system is characterized by a macroscopic number of Cooper pairs, *i.e.* that the expectation value of pairs is non-vanishing:

$$\Delta = \frac{g}{L^d} \sum_{\mathbf{k}} \langle \Omega_s | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | \Omega_s \rangle, \quad \bar{\Delta} = \frac{g}{L^d} \sum_{\mathbf{k}} \langle \Omega_s | c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} | \Omega_s \rangle \tag{6.38}$$

CMFT(6.17)

Δ assumes nonzero values below the transition temperature T_c, and vanishes above; it is therefore the **order parameter** of the SC transition (more details on this later).

The operator $c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}$ behaves like a creation operator for bosonic excitations. Nonvanishing expectation value for it: condensation.

In mean-field: express the operator as its mean value + small fluctuations,

$$\sum_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} = \frac{L^d}{g} \Delta + \left(\sum_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} - \frac{L^d}{g} \Delta \right) \tag{6.39}$$

and assume that the parentheses are small. The mean-field Hamiltonian then becomes (keeping only bilinears in electron operators)

$$\hat{H} - \mu \hat{N} \simeq \sum_{\mathbf{k}} \left[\xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - (\bar{\Delta} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + \Delta c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}) \right] + \frac{L^d}{g} |\Delta|^2 \tag{6.40}$$

which is known as the **Bogoliubov** or **Gor'kov** Hamiltonian, or **Bogoliubov-de Gennes** Hamiltonian in the West.

This Hamiltonian does **not** conserved electron number. To diagonalize it, introduce the **Nambu spinor** representation

$$\Psi^\dagger_{\mathbf{k}} = \begin{pmatrix} c^\dagger_{\mathbf{k}\uparrow} & c_{-\mathbf{k}\downarrow} \end{pmatrix}, \qquad \Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} \tag{6.41}$$

The Hamiltonian then becomes

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta \\ -\bar{\Delta} & -\xi_{\mathbf{k}} \end{pmatrix} \Psi_{\mathbf{k}} + \sum_{\mathbf{k}} \xi_{\mathbf{k}} + \frac{L^d}{g}|\Delta|^2. \tag{6.42}$$

This can be diagonalized by the unitary transformation

$$\chi_{\mathbf{k}} \equiv \begin{pmatrix} \alpha_{\mathbf{k}\uparrow} \\ \alpha^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} = \begin{pmatrix} \cos\theta_{\mathbf{k}} & \sin\theta_{\mathbf{k}} \\ \sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} \equiv U_{\mathbf{k}} \Psi_{\mathbf{k}} \tag{6.43}$$

which preserves the anticommutation relations of fermionic operators $\alpha_{\mathbf{k}\sigma}$ (exercise). Note: these operators combine creation and annihilation of original fermions !

Choose Δ to be real (gauge choice) and set $\tan 2\theta_{\mathbf{k}} = -\Delta/\xi_{\mathbf{k}}$. Defining

$$\lambda_{\mathbf{k}} = \sqrt{\Delta^2 + \xi^2_{\mathbf{k}}}, \tag{6.44}$$

CMFT(6.18)

we have $\cos 2\theta_{\mathbf{k}} = \xi_{\mathbf{k}}/\lambda_{\mathbf{k}}$ and $\sin 2\theta_{\mathbf{k}} = -\Delta/\lambda_{\mathbf{k}}$, and the Hamiltonian becomes

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}\sigma} \lambda_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}\sigma}\alpha_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - \lambda_{\mathbf{k}}) + \frac{L^d}{g}\Delta^2. \tag{6.45}$$

CMFT(6.19)

The elementary excitations (**Bogoliubov quasi-particles**) which are created by the $\alpha^\dagger$ operators therefore have an **energy gap** of Δ. Due to the gap, the ground state is 'rigid'.

The ground-state wavefunction is the vacuum state of the α operators,

$$\boxed{|\Omega_s\rangle \equiv \prod_{\mathbf{k}} \alpha_{\mathbf{k}\uparrow}\alpha_{-\mathbf{k}\downarrow}|0\rangle \sim \prod_{\mathbf{k}} (\cos\theta_{\mathbf{k}} - \sin\theta_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|0\rangle} \tag{6.46}$$

CMFT(6.19b)

with $\sin\theta_{\mathbf{k}} = \sqrt{1 - \xi_{\mathbf{k}}/\lambda_{\mathbf{k}}}$. Vacuum state: unique up to normalization. For $|\Omega_s\rangle$, the normalization is unity (exercise).

Final step: need to solve (6.38) CMFT(6.17) *self-consistently* for the parameter Δ:

$$\Delta = \frac{g}{L^d}\sum_{\mathbf{k}} \langle\Omega_s|c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}|\Omega_s\rangle = -\frac{g}{L^d}\sum_{\mathbf{k}} \sin\theta_{\mathbf{k}}\cos\theta_{\mathbf{k}} = \frac{g}{2L^d}\sum_{\mathbf{k}} \frac{\Delta}{(\Delta^2 + \xi^2_{\mathbf{k}})^{1/2}}$$
$$\simeq \frac{g\Delta}{2}\int_{-\omega_D}^{\omega_D} d\xi \frac{\nu(\xi)}{(\Delta^2 + \xi^2)^{1/2}} = g\Delta\nu \int_0^{\text{arcsinh }\omega_D/\Delta} dx = g\Delta\nu \,\text{arcsinh}(\omega_D/\Delta) \tag{6.47}$$

Assumptions made: density of states ν is roughly constant over energy scale ω_D, and interaction is also uniform.

We thus get

$$\boxed{\Delta = \frac{\omega_D}{\sinh(1/g\nu)} \simeq_{g\nu \ll 1} 2\omega_D e^{-\frac{1}{g\nu}}.} \tag{6.48}$$

CMFT(6.21)

Chapter 7

Response functions

RF

7. Response functions

Reminder: Schrödinger, Heisenberg and Interaction pictures

For a time-independent Hamiltonian H, the Schrödinger equation for states $|\psi^S(t)\rangle$ and its solution can be written

$$i\hbar\partial_t|\psi^S(t)\rangle = H|\psi^S(t)\rangle, \qquad |\psi^S(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi^S(t=0)\rangle \tag{7.1}$$

A time-dependent matrix element of some operator $\mathcal{O}^S$ thus reads

$$\langle\psi_1^S(t)|\mathcal{O}^S|\psi_2^S(t)\rangle \tag{7.2}$$

where states are time-dependent, and operators are time-independent. This is the **Schrödinger picture**.

In the **Heisenberg picture**, the time dependence is shifted from the states to the operators:

$$\langle\psi_1^S(t)|\mathcal{O}|\psi_2^S(t)\rangle = \langle\psi_1^S(t=0)|e^{\frac{i}{\hbar}Ht}\mathcal{O}^S e^{-\frac{i}{\hbar}Ht}|\psi_2^S(t=0)\rangle \equiv \langle\psi_1^H|\mathcal{O}^H(t)|\psi_2^H\rangle \tag{7.3}$$

in which states are time-independent,

$$|\psi^H\rangle \equiv |\psi^S(t=0)\rangle \tag{7.4}$$

and operators $\mathcal{O}^H(t) = e^{\frac{i}{\hbar}Ht}\mathcal{O}^S e^{-\frac{i}{\hbar}Ht}$ obey the equation of motion

$$\frac{d}{dt}\mathcal{O}^H(t) = \frac{i}{\hbar}\left[H, \mathcal{O}^H(t)\right] + e^{\frac{i}{\hbar}Ht}\partial_t\mathcal{O}^S e^{-\frac{i}{\hbar}Ht} \equiv \frac{i}{\hbar}\left[H, \mathcal{O}^H(t)\right] + \left[\partial_t\mathcal{O}\right]^H. \tag{7.5}$$

Let us now consider a generic, time-dependent Hamiltonian

$$H(t) = H_0 + V^S(t) \tag{7.6}$$

in which H_0 is the time-independent Hamiltonian of some exactly-solvable theory for which we know all the eigenstates, in other words for which we can provide a complete set of states $|\alpha^0\rangle$ such that

$$H_0|\alpha^0\rangle = E_{\alpha^0}|\alpha^0\rangle. \tag{7.7}$$

The operator $V^S(t)$ (in the Schrödinger representation) then represents some perturbation/additional interaction which we would like to take into account. The idea of the **interaction representation** is to 'Heisenbergize' using only H_0, meaning that we define states and operators as (here from their Schrödinger representation)

$$|\psi^I(t)\rangle = e^{\frac{i}{\hbar}H_0 t}|\psi^S(t)\rangle, \qquad \mathcal{O}^I(t) = e^{\frac{i}{\hbar}H_0 t}\mathcal{O}^S e^{-\frac{i}{\hbar}H_0 t}. \tag{7.8}$$

The time evolution of states in the interaction representation can be simply obtained from the Schrödinger equation as

$$i\hbar\partial_t|\psi^I(t)\rangle = e^{\frac{i}{\hbar}H_0 t}\left[-H_0 + H(t)\right]|\psi^S(t)\rangle = e^{\frac{i}{\hbar}H_0 t}V^S(t)|\psi^S(t)\rangle. \tag{7.9}$$

This can be simply rewritten as

$$i\hbar\partial_t|\psi^I(t)\rangle = V^I(t)|\psi^I(t)\rangle. \tag{7.10}$$ eq:SEIR

Thus, in the interaction representation, the change of the phase of a wavefunction is driven solely by the interaction term, and the time evolution of an operator is driven solely by the exactly-solvable part of the Hamiltonian.

Formally, one can write a solution to (7.10) as

$$|\psi^I(t)\rangle = U^I(t,t_0)|\psi^I(t_0)\rangle \tag{7.11}$$

in terms of the propagator U^I in the interaction representation. If $V^S(t)$ is in fact time-independent, we immediately have

$$U^I(t,t_0) = e^{\frac{i}{\hbar}H_0 t}e^{-\frac{i}{\hbar}H(t-t_0)}e^{-\frac{i}{\hbar}H_0 t_0}. \tag{7.12}$$

For a generic time-dependent $V^S(t)$, we have

$$i\hbar\partial_t U^I(t,t_0)|\psi^I(t_0)\rangle = V^I(t)U^I(t,t_0)|\psi^I(t_0)\rangle \tag{7.13}$$

so the propagator satisfies the equation (with obvious boundary condition)

$$i\hbar\partial_t U^I(t,t_0) = V^I(t)U^I(t,t_0), \qquad U^I(t_0,t_0) = 1. \tag{7.14}$$

We can write an iterative solution to this. Integrating from t_0 to t gives

$$U^I(t,t_0) = 1 + \frac{-i}{\hbar}\int_{t_0}^{t} dt' V^I(t')U^I(t',t_0) \tag{7.15}$$

so we can develop the perturbative series

$$U^I(t,t_0) = 1 + \frac{-i}{\hbar}\int_{t_0}^{t} dt' V^I(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 V^I(t_1)\int_{t_0}^{t_1} dt_2 V^I(t_2) + ... \tag{7.16}$$

This series can be represented as

$$\begin{aligned} U^I(t,t_0) &= \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 ... \int_{t_0}^{t_{n-1}} dt_n V^I(t_1)...V^I(t_n) \\ &= \sum_{n=0}^{\infty}\frac{(-i/\hbar)^n}{n!}\int_{t_0}^{t} dt_1...dt_n T_t\left[V^I(t_1)...V^I(t_n)\right] \end{aligned} \tag{7.17}$$

in which we have introduced the time-ordering operator T_t acting as (here, for $\mathcal{O}$ operators which are bosonic in character)

$$T_t\left[\mathcal{O}_1^I(t_1)\mathcal{O}_2^I(t_2)\right] \equiv \begin{cases} \mathcal{O}_1^I(t_1)\mathcal{O}_2^I(t_2), & t_1 > t_2 \\ \\ \mathcal{O}_2^I(t_2)\mathcal{O}_1^I(t_1), & t_1 < t_2 \end{cases} \tag{7.18}$$

(with straightforward generalization to an arbitrary product of operators at different times).

The propagator in the interaction representation is thus compactly represented as

$$U^I(t,t_0) = T_t\left[e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt' V^I(t')}\right]. \tag{7.19}$$

Reminder: Fermi's Golden Rule

Introducing some perturbation into a system generates some generally very complex time-dependent behaviour. One way to picture this time dependence is to still consider the original unperturbed basis of states, but have time-dependent state amplitudes. The probability of finding the system in a given state thus becomes time-dependent. For a small perturbation, the rates at which this probability flows from one state to another is given by **Fermi's Golden rule**.

Let us consider an exactly-solvable, time-independent Hamiltonian H_0 for which we know a basis of eigenstates

$$H_0|\alpha^0\rangle = E_{\alpha^0}|\alpha^0\rangle. \tag{7.20}$$

Let us consider perturbing this theory with a time-dependent operator which is adiabatically turned on from $t = -\infty$ onwards:

$$V(t) = Ve^{-i\omega t+\eta t}, \qquad \eta \to 0^+ \tag{7.21}$$

(we will evaluate this t for times much less than $1/\eta$). Here, V is some perturbing operator in the Schrödinger representation.

We now address the following question. If the initial state is

$$|\psi^S(t = t_0)\rangle = |\alpha_i^0\rangle \tag{7.22}$$

for some initial state $|\alpha_i^0\rangle$, what is the probability amplitude for finding the system in state $|\alpha_f^0\rangle$ (with $i \neq f$) at time t?

In the interaction representation, we had $|\psi^I(t)\rangle = U^I(t, t_0)|\psi^I(t_0)\rangle$. Since $|\psi^I(t)\rangle = e^{\frac{i}{\hbar}H_0 t}|\psi^S(t)\rangle$, we have $|\psi^I(t_0)\rangle = e^{\frac{i}{\hbar}H_0 t_0}|\alpha_i^0\rangle$ and thus

$$|\psi^S(t)\rangle = e^{-\frac{i}{\hbar}H_0 t}U^I(t, t_0)e^{\frac{i}{\hbar}H_0 t_0}|\alpha_i^0\rangle. \tag{7.23}$$

Consider now calculating the amplitude for being in state $|\alpha_f^0\rangle$, $f \neq i$, at time t:

$$\langle\alpha_f^0|\psi^S(t)\rangle = \langle\alpha_f^0|e^{-\frac{i}{\hbar}H_0 t}U^I(t, t_0)e^{\frac{i}{\hbar}H_0 t_0}|\alpha_i^0\rangle = e^{-\frac{i}{\hbar}E_{\alpha_f^0}t+\frac{i}{\hbar}E_{\alpha_i^0}t_0}\langle\alpha_f^0|U^I(t, t_0)|\alpha_i^0\rangle. \tag{7.24}$$

Using the series expansion for the propagator and keeping only the linear (in V) response, the matrix element of the propagator can be written

$$\langle\alpha_f^0|U^I(t, t_0)|\alpha_i^0\rangle = \langle\alpha_f^0|\alpha_i^0\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt'\langle\alpha_f^0|V^I(t')|\alpha_i^0\rangle + ... \tag{7.25}$$

The first term vanishes (we are looking for transition rates, so the initial and final states are different, $f \neq i$). The second term gives (substituting the explicit form of the perturbation)

$$-\frac{i}{\hbar}\int_{t_0}^{t} dt'\langle\alpha_f^0|e^{\frac{i}{\hbar}H_0 t'}V(t')e^{-\frac{i}{\hbar}H_0 t'}|\alpha_i^0\rangle = -\frac{i}{\hbar}\int_{t_0}^{t} dt' e^{\frac{i}{\hbar}[E_{\alpha_f^0}-E_{\alpha_i^0}-\hbar\omega-i\hbar\eta]t'}\langle\alpha_f^0|V|\alpha_i^0\rangle. \tag{7.26}$$

Since the matrix element is time-independent, we can perform the time integral, giving us

$$\langle\alpha_f^0|U^I(t, t_0)|\alpha_i^0\rangle = -\frac{\langle\alpha_f^0|V|\alpha_i^0\rangle}{E_{\alpha_f^0} - E_{\alpha_i^0} - \hbar\omega - i\hbar\eta}e^{\frac{i}{\hbar}[E_{\alpha_f^0}-E_{\alpha_i^0}-\hbar\omega-i\hbar\eta]t'}|_{t_0}^{t} + \mathrm{O}(V^2). \tag{7.27}$$

Let us now take the limit $t_0 \to -\infty$, with $\eta \to 0^+$ but $\eta t_0 \to -\infty$ while keeping t finite (that is, the perturbation is turned on at a vanishingly slow rate from the infinite past). This gives us

$$\langle\alpha_f^0|\psi^S(t)\rangle = \frac{\langle\alpha_f^0|V|\alpha_i^0\rangle}{\hbar\omega - (E_{\alpha_f^0} - E_{\alpha_i^0}) + i\eta\hbar}e^{-\frac{i}{\hbar}E_{\alpha_i^0}(t-t_0)}e^{-i\omega t+\eta t} + O(V^2). \tag{7.28}$$

The probability to be in state $|\alpha_f^0\rangle$ at time t, given that we initially started in state $|\alpha_i^0\rangle$ is thus

$$P_{f\leftarrow i}(t) = |\langle\alpha_f^0|\psi^S(t)\rangle|^2 = \frac{|\langle\alpha_f^0|V|\alpha_i^0\rangle|^2 e^{2\eta t}}{(\hbar\omega - (E_{\alpha_f^0} - E_{\alpha_i^0}))^2 + \eta^2\hbar^2}. \tag{7.29}$$

The rate at which this probability changes is thus

$$\frac{d}{dt}P_{f\leftarrow i}(t) = |\langle\alpha_f^0|V|\alpha_i^0\rangle|^2 \lim_{\eta\to 0^+} \frac{2\eta}{(\hbar\omega - (E_{\alpha_f^0} - E_{\alpha_i^0}))^2 + \eta^2\hbar^2}. \tag{7.30}$$

Using the representation of the Dirac delta function $\delta(x) = \lim_{\eta\to 0^+} \frac{1}{\pi}\frac{\eta}{x^2+\eta^2}$ then yields

Fermi's Golden rule	$\frac{d}{dt}P_{f\leftarrow i}(t) = \frac{2\pi}{\hbar}\|\langle\alpha_f^0\|V\|\alpha_i^0\rangle\|^2\delta(\hbar\omega - (E_{\alpha_f^0} - E_{\alpha_i^0}))$	(7.31)

Linear response theory

We can start our considerations by looking at a system represented by a Hamiltonian H_0, without having to specify in how many dimensions our system is, whether it is on the lattice or in the continuum, or what its operator content is. Let us imagine that we perturb our system by applying some external forces on it. We represent this by adding to the Hamiltonian a time-dependent term

$$H(t) = H_0 + F(t)\hat{P} \tag{7.32}$$

in which $\hat{P}$ is the (Hermitian) perturbing operator with which we connect to our system and F are the (real-valued) time-dependent parameters setting the scale of this change (this equation is in the Schrödinger picture, so $\hat{P}$ is time-independent).

What we are interested in is the effect of the presence of this perturbation on the expectation value which generic observables $\hat{O}$ take, that is we would like to calculate $\bar{O}(t) = \langle\psi(t)|\hat{O}|\psi(t)\rangle$. Generically, these expectation values will be complicated functionals of the applied perturbations.

Let us try to compute these expectation values using a minimal set of assumptions. Written in the interaction representation, such an expectation value becomes

$$\bar{O}(t) = \langle\psi^I(t)|\hat{O}^I(t)|\psi^I(t)\rangle = \langle\psi^I(t_0)|\left(U^I(t,t_0)\right)^{-1}\hat{O}^I(t)U^I(t,t_0)|\psi^I(t_0)\rangle \tag{7.33}$$

in which the propagator is (we put $\hbar = 1$ from now on)

$$U^I(t,t_0) = T_t\left[e^{-i\int_{t_0}^{t}dt'F(t')\hat{P}^I(t')}\right]. \tag{7.34}$$

Let us assume that the system starts in an eigenstate $|\psi_0\rangle$ of the unperturbed system at $t = t_0 = -\infty$, and that the perturbation parametrized by $F(t)$ is very small (the precise definition of 'very small' is actually quite complicated; for our purposes it suffices to say that it does not lead to modifications of order of one in the state occupation probability distribution). Expanding the propagator in powers of F allows to write

$$\bar{O}(t) = \bar{O}_{\psi_0} - i\int_{-\infty}^{t}dt'\langle\psi_0|[\hat{O}^I(t),\hat{P}^I(t')]|\psi_0\rangle F(t') + O(F^2) \tag{7.35}$$

in which $\bar{O}_{\psi_0} = \langle\psi_0|\hat{O}|\psi_0\rangle$ is the original expectation value in the unperturbed system. We now define the **retarded correlation function** (in eigenstate $|\psi\rangle$ of H_0) linking $\hat{P}$ and $\hat{O}$ as

$$\boxed{\mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi}(t-t') \equiv -i\theta(t-t')\langle\psi|[\hat{O}^I(t),\hat{P}^I(t')]|\psi\rangle} \tag{7.36}$$

in which the operators are in the interaction representation (*e.g.* $\hat{O}^I(t) = e^{iH_0t}\hat{O}e^{-iH_0t}$). Note that this in only a function of $t-t'$ (and not of the individual times) in view of our assumption that $|\psi\rangle$ is an eigenstate of H_0.

In terms of this, we find that in the presence of the perturbation $F(t)\hat{P}$, the expectation value of $\hat{O}$ obtains a linear correction as compared to its original, unperturbed value:

$$\boxed{\bar{O}(t) = \bar{O}_{\psi_0} + \int_{-\infty}^{\infty}dt'\mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi_0}(t-t')F(t') + O(F^2).} \tag{7.37}$$

This known as the **Kubo formula** and is the fundamental equation of **linear response theory**. Physically, the retarded function $\mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi_0}(t-t')$ thus connects a perturbation enforced by $\hat{P}$ acting at time t' to the modification of the value of $\bar{O}$ at time t. Since the retarded function vanishes for $t > t'$, only past perturbations can influence an expectation value, in other words the retarded function reflects the principle of causality.

The frequency-dependent retarded correlation function

Let us look more closely at our retarded correlation function. Setting $t' = 0$ without loss of generality, and expliciting the interaction representation for the operators, we get

$$\mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi_\alpha}(t) = -i\theta(t)\langle\psi_\alpha|\left(e^{iH_0t}\hat{O}e^{-iH_0t}\hat{P} - \hat{P}e^{iH_0t}\hat{O}e^{-iH_0t}\right)|\psi_\alpha\rangle. \tag{7.38}$$

Introducing a resolution of the identity $\mathbf{1} = \sum_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ between the two operators and defining the matrix elements

$$\langle\psi_\alpha|A|\psi_{\alpha'}\rangle \equiv A_{\alpha\alpha'} \tag{7.39}$$

we can write

$$\mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi_\alpha}(t) = -i\theta(t)\sum_{\alpha'}\left(O_{\alpha\alpha'}P_{\alpha'\alpha}e^{i(E_\alpha - E_{\alpha'})t} - P_{\alpha\alpha'}O_{\alpha'\alpha}e^{-i(E_\alpha - E_{\alpha'})t}\right). \tag{7.40}$$

Let us now introduce the Fourier transform (in time) of this retarded correlation function

$$\mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi_\alpha}(\omega) \equiv \int_{-\infty}^{\infty} dt\ \mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi_\alpha}(t)e^{i\omega t - \eta|t|} \tag{7.41}$$

in which we have introduced a regulator $\eta \to 0^+$ to ensure that the time integral converges. Performing this transform explicitly gives

$$\mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi_\alpha}(\omega) = \sum_{\alpha'}\left(\frac{O_{\alpha\alpha'}P_{\alpha'\alpha}}{\omega + E_\alpha - E_{\alpha'} + i\eta} - \frac{P_{\alpha\alpha'}O_{\alpha'\alpha}}{\omega - (E_\alpha - E_{\alpha'}) + i\eta}\right). \tag{7.42}$$

A representation such as this, where the time dependence has been explicitly extracted by using an eigenstate basis, is known as a **Lehmann representation**. Viewed as a function of the real frequency ω extended to complex values $\omega \in \mathbb{C}$, this retarded correlation function has singularities in (real) frequencies, which are at positions $\pm(E_\alpha - E_\beta) - i\eta$, in other words which are exclusively in the lower half-plane of ω. Any retarded correlation function is thus analytic in the upper half-plane of such a (generically complex-valued) ω.

Note that introducing $\eta \to 0$ is purely a convenience trick to make calculations easily tractable. Without it, we would for example have to deal with integrals of the form

$$\int_{-\infty}^{\infty} dt\theta(t)e^{i(\omega - E)t} = \int_0^{\infty} dte^{i(\omega - E)t} \tag{7.43}$$

which are ill-defined as they stand. On the other hand, with the regulator, they become trivial:

$$-i\int_0^{\infty} dte^{i(\omega - E)t - \eta t} = \frac{1}{\omega - E + i\eta}. \tag{7.44}$$

The physical interpretation which can be given to the regulator is that it represents generic decoherence between wavefunctions at large times: quantum oscillations between states don't remain phase coherent forever, leading to the eventual decay (in time) of correlations. To separate the real and imaginary parts of a correlator, we can make use of a particularly useful identity due to Dirac:

$$\lim_{\eta\to 0^+}\frac{1}{\omega \pm i\eta} = \mp i\pi\delta(\omega) + P\frac{1}{\omega} \tag{7.45}$$

in which P represents taking the principal part of the integral in which this function stands.

Advanced and real-time correlation functions

Besides the retarded correlation function, it is also possible to define the following functions: the **advanced correlation function** which (contrary to the retarded function) is only nonvanishing for negative time arguments,

$$\mathcal{C}^{\hat{O},\hat{P}}_{adv,\psi}(t-t') \equiv i\theta(t'-t)\langle\psi|[\hat{O}^I(t),\hat{P}^I(t')]|\psi\rangle \tag{7.46}$$

or (taking again $t'=0$ without loss of generality)

$$\mathcal{C}^{\hat{O},\hat{P}}_{adv,\psi_\alpha}(t) = i\theta(-t)\sum_{\alpha'}\left(O_{\alpha\alpha'}P_{\alpha'\alpha}e^{i(E_\alpha-E_{\alpha'})t} - P_{\alpha\alpha'}O_{\alpha'\alpha}e^{-i(E_\alpha-E_{\alpha'})t}\right). \tag{7.47}$$

Under the (time) Fourier transform (using the same conventions as for the retarded function), this becomes

$$\mathcal{C}^{\hat{O},\hat{P}}_{adv,\psi_\alpha}(\omega) = \sum_{\alpha'}\left(\frac{O_{\alpha\alpha'}P_{\alpha'\alpha}}{\omega+E_\alpha-E_{\alpha'}-i\eta} - \frac{P_{\alpha\alpha'}O_{\alpha'\alpha}}{\omega-(E_\alpha-E_{\alpha'})-i\eta}\right) \tag{7.48}$$

so the advanced function is analytic in complex ω in the entire lower-half plane.

We can also define the **real-time correlation function** involving the time-ordered product of the operators,

$$\mathcal{C}^{\hat{O},\hat{P}}_{\psi}(t-t') \equiv -i\langle\psi|T_t(\hat{O}^I(t)\hat{P}^I(t'))|\psi\rangle \tag{7.49}$$

or equivalently

$$\mathcal{C}^{\hat{O},\hat{P}}_{\psi_\alpha}(t) = -i\sum_{\alpha'}\left(O_{\alpha\alpha'}P_{\alpha'\alpha}\;\theta(t)e^{i(E_\alpha-E_{\alpha'})t} + P_{\alpha\alpha'}O_{\alpha'\alpha}\;\theta(-t)e^{-i(E_\alpha-E_{\alpha'})t}\right). \tag{7.50}$$

The (time) Fourier transform of the real-time correlation function can thus be written

$$\mathcal{C}^{\hat{O},\hat{P}}_{\psi_\alpha}(\omega) = \sum_{\alpha'}\left(\frac{O_{\alpha\alpha'}P_{\alpha'\alpha}}{\omega+E_\alpha-E_{\alpha'}+i\eta} - \frac{P_{\alpha\alpha'}O_{\alpha'\alpha}}{\omega-(E_\alpha-E_{\alpha'})-i\eta}\right) \tag{7.51}$$

and is not analytic either in the lower or upper half-plane of ω.

Thermal correlation functions

Up to now, we have written out correlation functions for a given specific initial state. More generally, if the initial condition is represented by an ensemble, the correlation function can be written as (here the retarded function for a Gibbs ensemble; advanced and real-time correlations are defined in a similar manner)

$$\mathcal{C}^{\hat{O},\hat{P}}_{ret}(t) = \frac{1}{\mathcal{Z}}\sum_\alpha \mathcal{C}^{\hat{O},\hat{P}}_{ret,\psi_\alpha}(t)e^{-\beta E_\alpha} = -i\frac{\theta(t)}{\mathcal{Z}}\sum_\alpha\langle\psi_\alpha|[\hat{O}^I(t),\hat{P}^I(0)]|\psi_\alpha\rangle e^{-\beta E_\alpha}, \tag{7.52}$$

with partition function (note: if you are working in a grand canonical ensemble, you can view the chemical potential as being included in the definition of E_α)

$$\mathcal{Z} = \sum_\alpha e^{-\beta E_\alpha}. \tag{7.53}$$

Performing the same computations as above (using the Lehmann representation), and interchanging indices in the second sum, we obtain

$$\mathcal{C}^{\hat{O},\hat{P}}_{ret}(\omega) = \frac{1}{\mathcal{Z}} \sum_{\alpha,\alpha'} O_{\alpha\alpha'} P_{\alpha'\alpha} \frac{e^{-\beta E_\alpha} - e^{-\beta E_{\alpha'}}}{\omega + E_\alpha - E_{\alpha'} + i\eta} \tag{7.54}$$

eq:Creteq

$$\mathcal{C}^{\hat{O},\hat{P}}_{adv}(\omega) = \frac{1}{\mathcal{Z}} \sum_{\alpha,\alpha'} O_{\alpha\alpha'} P_{\alpha'\alpha} \frac{e^{-\beta E_\alpha} - e^{-\beta E_{\alpha'}}}{\omega + E_\alpha - E_{\alpha'} - i\eta} \tag{7.55}$$

$$\mathcal{C}^{\hat{O},\hat{P}}(\omega) = \frac{1}{\mathcal{Z}} \sum_{\alpha,\alpha'} O_{\alpha\alpha'} P_{\alpha'\alpha} \left(\frac{e^{-\beta E_\alpha}}{\omega + E_\alpha - E_{\alpha'} + i\eta} - \frac{e^{-\beta E_{\alpha'}}}{\omega + E_\alpha - E_{\alpha'} - i\eta} \right) \tag{7.56}$$

The analytic structure thus remains the same at finite temperature: the retarded (advanced) function has singularities in the lower (upper) half-plane, whereas the real-time correlation function has singularities in both half-planes.

The imaginary-time correlation function

Besides the definitions of correlations in real time provided above, it is also convenient to define the **imaginary-time** (thermal equilibrium) correlation function as

$$\mathcal{C}^{\hat{O},\hat{P}}_{\tau}(\tau_1 - \tau_2) \equiv -\langle T_\tau(\hat{O}(\tau_1)\hat{P}(\tau_2))\rangle \tag{7.57}$$

in which $\langle(...)\rangle$ means thermal averaging and T_τ is the imaginary-time ordering operator (acting in a similar manner to the real-time ordering operator T_t), and in which we have used the imaginary-time interaction (in other words Heisenberg for the Hamiltonian H_0) representation

$$\hat{O}(\tau) \equiv e^{\tau \hat{H}_0} \hat{O} e^{-\tau \hat{H}_0}. \tag{7.58}$$

In the Lehmann representation, this becomes

$$\mathcal{C}^{\hat{O},\hat{P}}_{\tau}(\tau) = -\frac{1}{\mathcal{Z}} \sum_{\alpha,\alpha'} O_{\alpha\alpha'} P_{\alpha'\alpha} e^{(E_\alpha - E_{\alpha'})\tau} \left(\theta(\tau) e^{-\beta E_\alpha} + \theta(-\tau) e^{-\beta E_{\alpha'}} \right), \quad \tau \in]-\beta, \beta[\tag{7.59}$$

(the argument's restriction to $]-\beta, \beta[$ coming from the fact that it's really $\tau_1 - \tau_2$ with $\tau_i \in [0, \beta[$). By inspection, this has the periodicity property

$$\mathcal{C}^{\hat{O},\hat{P}}_{\tau}(\tau) = \mathcal{C}^{\hat{O},\hat{P}}_{\tau}(\tau + \beta), \qquad -\beta < \tau < 0 \tag{7.60}$$

so this correlation function has a Fourier transformation in imaginary-time with (bosonic) Matsubara frequencies $i\omega_n$ according to $\mathcal{C}(i\omega_n) = \int_0^\beta d\tau \mathcal{C}(\tau) e^{i\omega_n \tau}$. Performing this Fourier transform gives

$$\mathcal{C}^{\hat{O},\hat{P}}_{\tau}(i\omega_n) = \sum_{\alpha,\alpha'} O_{\alpha\alpha'} P_{\alpha'\alpha} \frac{e^{-\beta E_\alpha} - e^{-\beta E_{\alpha'}}}{i\omega_n + E_\alpha - E_{\alpha'}}. \tag{7.61}$$

Comparing with (7.54) eq:Creteq shows that the imaginary-time and (real-time) (thermal equilibrium) retarded correlation functions are related by the formal analytic continuation

$$\mathcal{C}^{\hat{O},\hat{P}}_{ret}(\omega) = \mathcal{C}^{\hat{O},\hat{P}}_{\tau}(i\omega_n)|_{i\omega_n \to \omega + i\eta}. \tag{7.62}$$

Defining the 'master function'

$$\mathcal{C}_\tau^{\hat{O},\hat{P}}(z) = \sum_{\alpha,\alpha'} O_{\alpha\alpha'} P_{\alpha'\alpha} \frac{e^{-\beta E_\alpha} - e^{-\beta E_{\alpha'}}}{z + E_\alpha - E_{\alpha'}} \tag{7.63}$$

for generic complex argument z, we have that $\mathcal{C}_{ret}, \mathcal{C}_{adv}, \mathcal{C}_\tau$ are respectively given by taking $z \to \omega + i\eta$, $\omega - i\eta$, $i\omega_n$. By inspection, $C(z)$ is analytic everywhere except on the real axis. Suppose that we somehow have managed to compute $\mathcal{C}_\tau(i\omega_n)$ for all positive Matsubara frequencies $i\omega_{n>0}$, and that we can find the analytic continuation of $\mathcal{C}(z)$ to the upper half-plane $\Im(z) > 0$. The retarded correlation function would then be given by the evalution of this function on the shifted real axis $z = \omega + i\eta$.

Single-particle correlation functions

Up to now, we have considered generic hermitian operators $\hat{P}$ and $\hat{O}$ respectively effectuating the perturbation and representing the observable of interest. These can be composite, many-body operators, which can be written in terms of the fundamental creation and annihilation operators in our theory, which can be either bosonic or fermionic. Since everything can (at least in principle) be rewritten in terms of (higher-point) correlations of these fundamental operators, let us now specialize to the case of one-body (or single-particle) correlation functions.

The simplest example: free fermions

Let us consider the very simplest case possible: free particles in a translationally-invariant system. Our Hamiltonian is thus diagonalized in Fourier modes as

$$H_0 = \sum_k \varepsilon_k a_k^\dagger a_k \tag{7.64}$$

with $[a_k, a_{k'}^\dagger] = \delta_{k,k'}$.

Retarded function. The single-particle retarded correlation function (in state $|\psi\rangle$) is then defined as

$$\mathcal{C}^{ret}_{\beta,\mu;k}(t_1 - t_2) = -i\theta(t_1 - t_2)\langle\Big\{a_k(t_1), a_k^\dagger(t_2)\Big\}\rangle_{\beta,\mu} \tag{7.65}$$

with $\{,\}$ denoting the anticommutator and where the equilibrium thermal average at fixed (inverse) temperature and chemical potential is denoted

$$\langle(...)\rangle_{\beta,\mu} \equiv \frac{1}{\mathcal{Z}_{\beta,\mu}} \sum_\alpha (...) e^{-\beta(E_\alpha - \mu N_\alpha)}, \qquad \mathcal{Z}_{\beta,\mu} \equiv \sum_\alpha e^{-\beta(E_\alpha - \mu N_\alpha)}. \tag{7.66}$$

Introducing a resolution of the identity and using the interaction representation in the grand-canonical ensemble (so including the chemical potential specifically)

$$a_k(t) = e^{i(H_0 - \mu N)t} a_k e^{-i(H_0 - \mu N)t} = e^{-i\xi_k t} a_k, \qquad a_k^\dagger(t) = e^{i\xi_k t} a_k^\dagger, \qquad \xi_k \equiv \varepsilon_k - \mu \tag{7.67}$$

we can rewrite the retarded correlator as

$$\mathcal{C}^{ret}_{\beta,\mu;k}(t_1 - t_2) = -i\theta(t_1 - t_2) e^{-i\xi_k(t_1 - t_2)} \Big(\langle a_k a_k^\dagger\rangle_{\beta,\mu} + \langle a_k^\dagger a_k\rangle_{\beta,\mu}\Big) \tag{7.68}$$

Since the occupation of fermions is simply the Fermi distribution, we immediately have

$$\langle a_k^\dagger a_k\rangle_{\beta,\mu} = n_F(\xi_k;\beta) \tag{7.69}$$

and our retarded function simplifies to

$$\mathcal{C}^{ret}_{\beta,\mu;k}(t_1 - t_2) = -i\theta(t_1 - t_2) e^{-i\xi_k(t_1 - t_2)}. \tag{7.70}$$

Fourier transforming (in time) using

$$\mathcal{C}(\omega) \equiv \int_{-\infty}^{\infty} dt e^{i\omega t - \eta|t|}\, \mathcal{C}(t) \tag{7.71}$$

gives

$$\mathcal{C}^{ret}_{\beta,\mu;k}(\omega) = \frac{1}{\omega - \xi_k + i\eta}. \tag{7.72}$$

The advanced function. The advanced function is defined as

$$\mathcal{C}^{adv}_{\beta,\mu;k}(t_1 - t_2) = i\theta(t_2 - t_1)\langle\Big\{a_k(t_1), a_k^\dagger(t_2)\Big\}\rangle_{\beta,\mu} \tag{7.73}$$

and takes the simple form

$$\mathcal{C}^{adv}_{\beta,\mu;k}(t_1 - t_2) = i\theta(t_2 - t_1)e^{-i\xi_k(t_1-t_2)}. \tag{7.74}$$

Fourier tranforming to frequency, this is

$$\mathcal{C}^{adv}_{\beta,\mu;k}(\omega) = \frac{1}{\omega - \xi_k - i\eta}. \tag{7.75}$$

Note that the advanced and retarded functions are here linked by simple conjugation:

$$\mathcal{C}^{adv}_{\beta,\mu;k}(\omega) = (\mathcal{C}^{ret}_{\beta,\mu;k}(\omega))^*, \qquad \omega \in \mathbb{R}. \tag{7.76}$$

Other useful real-time-dependent functions. In addition to the retarded and advanced functions, the following two functions (the 'greater' and 'lesser' functions) are useful to define:

$$\mathcal{C}^{>}_{\beta,\mu;k}(t_1 - t_2) = -i\langle a_k(t_1)a_k^\dagger(t_2)\rangle_{\beta,\mu}, \tag{7.77}$$

$$\mathcal{C}^{<}_{\beta,\mu;k}(t_1 - t_2) = -i\zeta\langle a_k^\dagger(t_2)a_k(t_1)\rangle_{\beta,\mu}. \tag{7.78}$$

These are simply related to the retarded and advanced functions as

$$\begin{aligned}\mathcal{C}^{ret}(t - t') &= \theta(t - t')\left(\mathcal{C}^{>}(t - t') - \mathcal{C}^{<}(t - t')\right)\\ \mathcal{C}^{adv}(t - t') &= \theta(t' - t)\left(\mathcal{C}^{<}(t - t') - \mathcal{C}^{>}(t - t')\right).\end{aligned} \tag{7.79}$$

A direct calculation similar to that given for the retarded function gives (for our free fermions)

$$\begin{aligned}\mathcal{C}^{>}_{\beta,\mu;k}(t - t') &= -i(1 - n_F(\xi_k;\beta))e^{-i\xi_k(t-t')},\\ \mathcal{C}^{<}_{\beta,\mu;k}(t - t') &= in_F(\xi_k;\beta)e^{-i\xi_k(t-t')}.\end{aligned} \tag{7.80}$$

Imaginary-time correlation function. The retarded function is simply related to the imaginary-time correlation

$$\mathcal{C}^{\tau}_{\beta,\mu;k}(i\omega_n) = \frac{1}{i\omega_n - \xi_k} \tag{7.81}$$

by performing the analytic continuation $i\omega_n \to \omega + i\eta$.

The spectral function. A particularly meaningful quantity is the **single-particle spectral function** defined simply as

$$A_{\beta,\mu;k}(\omega) = -2\ \mathrm{Im}\ (\mathcal{C}^{ret}_{\beta,\mu;k}(\omega)). \tag{7.82}$$

The greater and lesser functions are related to the spectral function according to

$$\mathcal{C}^{>}_{\beta,\mu;k}(\omega) = -i(1 - n_F(\omega - \mu;\beta))A_{\beta,\mu;k}(\omega), \qquad \mathcal{C}^{<}_{\beta,\mu;k}(\omega) = in_F(\omega - \mu;\beta)A_{\beta,\mu;k}(\omega). \tag{7.83}$$

As can be shown from the Lehmann representation, the spectral function is also related to the retarded and advanced functions as

$$\mathcal{C}^{ret}_{\beta,\mu;k}(\omega) = \int \frac{d\omega'}{2\pi}\frac{A_{\beta,\mu;k}(\omega')}{\omega - \omega' + i\eta}, \qquad \mathcal{C}^{adv}_{\beta,\mu;k}(\omega) = \int \frac{d\omega'}{2\pi}\frac{A_{\beta,\mu;k}(\omega')}{\omega - \omega' - i\eta}. \tag{7.84}$$

For free fermions, using the Dirac identity, the spectral function simply becomes

$$A_{\beta,\mu;k}(\omega) = 2\pi\delta(\omega - \xi_k). \tag{7.85}$$

Appendix A

Prerequisites

PRE

A.1 Mathematics

PRE:Math

Fourier transformations

In the continuum. Let $f(x)$ be an integrable function of a real parameter x, which satisfies $\int_{-\infty}^{\infty} dx|f(x)| < \infty$. It can be represented as a Fourier transform:

$$\boxed{f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} f(k)} \quad \text{with coefficients} \quad \boxed{f(k) = \int_{-\infty}^{\infty} dx e^{-ikx} f(x)} \tag{A.1}$$

To go from one representation to the other, one uses the identity

$$\boxed{\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x_0)} = \delta(x - x_0)} \tag{A.2}$$

Continuum, finite interval. Let $f(x)$ be an integrable function defined on a finite interval $x \in [0, L[$. If we extend the definition of $f(x)$ to the whole real line by assuming (quasi-)periodicity $f(x + L) = e^{i2\pi\alpha} f(x)$ for some $\alpha \in [0, 1[$, we can represent $f(x)$ as the Fourier series

$$\boxed{f(x) = \frac{1}{L} \sum_{n\in\mathbb{Z}} e^{ik_n x} f_{k_n}}, \quad \boxed{f_{k_n} = \int_0^L dx e^{-ik_n x} f(x)} \quad \text{where} \quad \boxed{k_n \equiv \frac{2\pi}{L}(n + \alpha)} \tag{A.3}$$

To go from one representation to the other, one uses the identities

$$\boxed{\frac{1}{L} \sum_{n\in\mathbb{Z}} e^{ik_n(x-x_0)} = \sum_{m\in\mathbb{Z}} \delta(x - x_0 - mL)}, \qquad \boxed{\int_0^L dx e^{i(k_n - k_m)x} = L\delta_{n,m}} \tag{A.4}$$

The infinite-size limit is easily recovered by using the replacement $\frac{1}{L}\sum_n \to \int_{-\infty}^{\infty} \frac{dk}{2\pi}$.

Finite lattice. Consider a lattice of N points labeled by index $j = 1, ..., N$. We denote the lattice spacing by a. Let f_j be a number associated to site j. Assuming again some (quasi-

)periodicity $f_{j+N} = e^{i2\pi\alpha} f_j$, the Fourier series can be defined as (other conventions are possible)

$$\boxed{f_j = \frac{1}{N} \sum_{k_n \in \text{ BZ}} e^{ik_n aj} f_{k_n}}, \qquad \boxed{f_{k_n} = \sum_{j=1}^{N} e^{-ik_n aj} f_j}, \qquad \boxed{k_n \equiv \frac{2\pi}{Na}(n+\alpha)} \tag{A.5}$$

To go from one representation to the other, you can use the identities

$$\boxed{\frac{1}{N} \sum_{k_n \in \text{ BZ}} e^{ik_n a(j-l)} = \delta_{j,l}}, \qquad \boxed{\sum_{j=1}^{N} e^{-i(k_n - k_m)aj} = N\delta_{n,m}} \tag{A.6}$$

The notation $k_n \in$ BZ means that we sum the momenta over one Brillouin zone, for example by convention by choosing $n = -N/2+1, -N/2+2, ..., N/2$ (for N even) or $n = 0, ..., N-1$, which respectively become $k \in]-\pi/a, \pi/a]$ and $k \in [0, 2\pi/a[$ in the infinite lattice size limit. In the continuum limit $a \to 0$, we simply redefine $Na \to L$, $aj \to x$ and $f_j \to af(x)$, and use the rule $a\sum_{j=1}^{N}(...) \to \int_0^L dx(...)$ to fall back onto the earlier formulas.

Note that very often, the prefactors $\frac{1}{2\pi}$, $\frac{1}{N}$ or $\frac{1}{L}$ are 'shared' between the direct and inverse Fourier transforms. You can then (like in the CMFT book) encounter expressions like

$$f_j = \frac{1}{\sqrt{N}} \sum_{k_n \in \text{ BZ}} e^{ik_n aj} \tilde{f}_{k_n}, \qquad \tilde{f}_{k_n} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-ik_n aj} f_j. \tag{A.7}$$

This is only a matter of convention, and should be clear from the context. The only important thing is that the *product* of prefactors equals $\frac{1}{N}$ (for the case of a finite lattice), $\frac{1}{L}$ (for the finite continuum interval) or $\frac{1}{2\pi}$ (for the infinite continuum).

The multidimensional cases are straightforward generalizations of the above formulas.

Taylor expansions

Let $f(x)$ be a function of a real parameter x. If f is infinitely differentiable around a point x_0, its Taylor series is given by

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n, \qquad f^{(n)}(x_0) \equiv \left.\frac{d^n f(x)}{dx^n}\right|_{x=x_0}. \tag{A.8}$$

Dirac δ function (distribution[1])

$$\delta(x) = \begin{cases} \infty & x = 0, \\ 0 & x \neq 0, \end{cases} \qquad \text{such that} \qquad \int dx f(x)\delta(x - x_0) = f(x_0) \tag{A.9}$$

for $f(x)$ a continuous function of a real parameter x.

Laurent series

The Laurent series of a function $f(z)$ of a complex parameter $z \in \mathbb{C}$ is a generalization of the Taylor series, including negative powers:

$$f(z) = \sum_{n=-\infty}^{\infty} f_n (z - z_0)^n. \tag{A.10}$$

The coefficient f_{-1} is called the complex residue of f at z_0. The coefficients f_n are obtained from the contour integral

$$f_n = \frac{1}{2\pi i} \oint_\gamma dz \frac{f(z)}{(z - z_0)^{n+1}} \tag{A.11}$$

in which γ is a counterclockwise closed curve enclosing z_0.

Cauchy's residue theorem

Let $f(z)$ be a holomorphic function in the complex plane, except at isolated poles z_i. Then,

$$\frac{1}{2\pi i} \oint_\gamma dz f(z) = \sum_{z_i \in \gamma} \mathrm{Res}_f(z_i) \tag{A.12}$$

where $\mathrm{Res}_f(z_i)$ is the residue of f at z_i, and the sum is taken over all z_i inside the (counterclockwise) closed curve γ.

[1] For the finicky among you.

Gaussian integration

Review of Gaussian integration One-dimensional Gaussian integral:

$$I(a) \equiv \int_{-\infty}^{\infty} dx e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}, \qquad \Re a > 0. \tag{A.13}$$ CMFT(3.9)

First moment:

$$\int_{-\infty}^{\infty} dx x^2 e^{-\frac{a}{2}x^2} = -2\partial_a I(a) = \sqrt{\frac{2\pi}{a^3}}. \tag{A.14}$$

With linear piece:

$$\int_{-\infty}^{\infty} dx e^{-\frac{a}{2}x^2+bx} = \int_{-\infty}^{\infty} dx e^{-\frac{a}{2}(x-b/a)^2+\frac{b^2}{2a}} = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}}, \qquad b \in \mathbb{C}. \tag{A.15}$$ CMFT(3.10)

Generalization to complex arguments: for $z = x + iy$, $\int d(\bar{z}, z) = \int_{-\infty}^{\infty} dxdy$,

$$\int d(\bar{z}, z) e^{-\bar{z}wz} = \frac{\pi}{w}, \qquad \Re w > 0. \tag{A.16}$$

and

$$\int d(\bar{z}, z) e^{-\bar{z}wz+\bar{u}z+\bar{z}v} = \frac{\pi}{w} e^{\frac{\bar{u}v}{w}}, \qquad \Re w > 0. \tag{A.17}$$ CMFT(3.11)

Gaussian integration in more than one dimension: real case

$$\int d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}} = (2\pi)^{N/2} \det \mathbf{A}^{-1/2} \tag{A.18}$$ CMFT(3.12)

where $\mathbf{A}$ is a positive definite[2] real symmetric N-dimensional matrix and $\mathbf{v}$ is an N-component real vector.

Proof: can write $\mathbf{A} = \mathbf{O}^T\mathbf{D}\mathbf{O}$ with $\mathbf{O}$ an orthogonal matrix and $\mathbf{D}$ a diagonal matrix. Change of variables $\mathbf{v} \to \mathbf{O}\mathbf{v}$ having unit Jacobian $\det\mathbf{O} = 1$. Factorizes into product of one-dimensional Gaussian integrals, result $\prod_{i=1}^{N} \sqrt{\frac{2\pi}{d_i}}$. Replace product by determinant.

Multidimensional generalization of (A.15): CMFT(3.10)

$$\int d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}+\mathbf{j}^T\cdot\mathbf{v}} = (2\pi)^{N/2} \det \mathbf{A}^{-1/2} e^{\frac{1}{2}\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}} \tag{A.19}$$ CMFT(3.13)

This is important as a 'generator' of other useful identities.

Applying $\partial^2_{j_m j_n}|_{\mathbf{j}=0}$ to LHS of (A.19) gives $\int d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}} v_m v_n = (2\pi)^{N/2} \det \mathbf{A}^{-1/2} A^{-1}_{mn}$ or CMFT(3.13)

$$\langle v_m v_n \rangle = A^{-1}_{mn} \tag{A.20}$$ CMFT(3.14)

with

$$\langle ... \rangle \equiv (2\pi)^{-N/2} \det \mathbf{A}^{1/2} \int d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}} (...) \tag{A.21}$$ CMFT(3.15)

[2]The matrix A is positive definite if $\mathbf{v}^T A\mathbf{v}$ is positive for any nonzero real vector $\mathbf{v}$.

This generalizes: differentiating four times,

$$\langle v_m v_n v_q v_p \rangle = A^{-1}_{mn} A^{-1}_{qp} + A^{-1}_{mq} A^{-1}_{np} + A^{-1}_{mp} A^{-1}_{nq} \tag{A.22}$$

$2n$-fold differentiation:

$$\langle v_{i_1} v_{i_2} ... v_{i_{2n}} \rangle = \sum_{pairings} A^{-1}_{i_{k_1} i_{k_2}} ... A^{-1}_{i_{k_{2n-1}} i_{k_{2n}}} \tag{A.23}$$ CMFT(3.16)

which is known as **Wick's theorem**, here for real bosonic fields. Total number of terms: $C_{2n} = \frac{(2n)!}{n! 2^n} = (2n-1)!!$, *i.e.* using pair exchange symmetry and exchange symmetry within each pair.

Gaussian integration in more than one dimension: complex case Complex version of (CMFT(3.12) A.18):

$$\int d(\mathbf{v}^\dagger, \mathbf{v}) e^{-\mathbf{v}^\dagger \mathbf{A} \mathbf{v}} = \pi^N \det \mathbf{A}^{-1} \tag{A.24}$$ CMFT(3.17)

with $\mathbf{v}$ an N-dimensional complex vector, $d(\mathbf{v}^\dagger, \mathbf{v}) \equiv \prod_{i=1}^N d\Re v_i d\Im v_i$, and $\mathbf{A}$ a complex matrix with positive definite Hermitian part.

Generalization of (CMFT(3.17) A.24):

$$\int d(\mathbf{v}^\dagger, \mathbf{v}) e^{-\mathbf{v}^\dagger \mathbf{A} \mathbf{v} + \mathbf{w}^\dagger \cdot \mathbf{v} + \mathbf{v}^\dagger \cdot \mathbf{w}'} = \pi^N \det \mathbf{A}^{-1} e^{\mathbf{w}^\dagger \mathbf{A}^{-1} \mathbf{w}'} \tag{A.25}$$ CMFT(3.18)

with $\mathbf{w}, \mathbf{w}'$ independent vectors in general.

Averages of components: differentiating this twice, $\partial^2_{w'_m \bar{w}_n}(...)|_{\mathbf{w}=\mathbf{w}'=0}$ gives

$$\langle \bar{v}_m v_n \rangle = A^{-1}_{nm} \tag{A.26}$$

where $\langle ... \rangle \equiv \pi^{-N} \det \mathbf{A} \int d(\mathbf{v}^\dagger, \mathbf{v}) e^{-\mathbf{v}^\dagger \mathbf{A} \mathbf{v}} (...)$.

For $2n$ components: Wick's theorem for complex bosonic fields:

$$\langle \bar{v}_{i_1} \bar{v}_{i_2} ... \bar{v}_{i_n} v_{j_1} v_{j_2} ... v_{j_n} \rangle = \sum_P A^{-1}_{j_1 i_{P_1}} ... A^{-1}_{j_n i_{P_n}} . \tag{A.27}$$

Total number of terms: $C_n = n!$.

A.2 Physics

PRE:Phys

Lagrangian and Hamiltonian mechanics

Recap of the principle of least action for a single point particle

Let $L(x, \dot{x})$ be the classical Lagrangian of a point particle, and $S[x] = \int dt L(x, \dot{x})$. The **principle of least action** states that the path $x(t)$ realized by the particle is the one which extremizes the action, $\delta S[x] = 0$, meaning that for any curve $t \mapsto y(t)$,

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon}(S[x + \epsilon y] - S[x]) = 0. \tag{A.28}$$

CMFT(1.6)

This is fulfilled if and only if $x(t)$ satisfies **Lagrange's equation of motion**

$$\frac{d}{dt}(\partial_{\dot{x}} L) - \partial_x L = 0. \tag{A.29}$$

CMFT(1.7)

Check:

$$\begin{aligned} S[x + \epsilon y] - S[x] &= \int dt (L(x + \epsilon y, \dot{x} + \epsilon \dot{y}) - L(x, \dot{x})) \\ &= \epsilon \int dt ((\partial_x L(x, \dot{x}))y + (\partial_{\dot{x}} L(x, \dot{x}))\dot{y}) + O(\epsilon^2) \\ = \epsilon \int dt ((\partial_x L(x, \dot{x})) - \frac{d}{dt}(\partial_{\dot{x}} L(x, \dot{x})))y + ((\partial_{\dot{x}} L)y)|_0^t + O(\epsilon^2) \end{aligned} \tag{A.30}$$

The second step uses partial integration. The variation $y(t)$ is assumed to vanish at the boundary points[3], so the boundary terms vanish. Since (CMFT(1.6) A.28) is taken to hold true for any y satisfying these boundary conditions, (CMFT(1.7) A.29) is obtained for any t.

Statistical mechanics

The partition function of a system is given by

$$\mathcal{Z} = \sum_\alpha e^{-\beta(H_\alpha - \mu N_\alpha)} \tag{A.31}$$

where β is the inverse temperature, μ is the chemical potential, and α labels (eigen)states.

Quantum harmonic oscillator

Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 \tag{A.32}$$

Energy levels: $\varepsilon_n = \omega(n + 1/2)$, wavefunctions are Hermite polynomials, *e.g.*
$\Psi_0(x) = (m\omega/\hbar\pi)^{1/4} e^{-m\omega x^2/2\hbar}$.

Ladder operators:

$$\hat{a} \equiv \sqrt{\frac{m\omega}{2}}(\hat{x} + \frac{i}{m\omega}\hat{p}), \qquad \hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2}}(\hat{x} - \frac{i}{m\omega}\hat{p}) \tag{A.33}$$

[3]Here, we haven't specified any boundary conditions (for example, periodic), so we put the variation to zero at the system's ends.

with canonical commutation relations

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{A.34}$$ CMFT(1.30)

Operator form of Hamiltonian:

$$\hat{H} = \omega(\hat{a}^\dagger \hat{a} + 1/2) \tag{A.35}$$ CMFT(1.31)

Vacuum state ($\equiv$ ground state): $|0\rangle$ such that $\hat{a}|0\rangle = 0$. Complete hierarchy of states: $|n\rangle \equiv \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle$.

Bloch's theorem

Imagine that we're trying to describe the behaviour of electrons in a solid in the language of quantum mechanics. Since the ions in a crystal can in a first approximation considered to be fixed in place, the electrons move in a potential $U(\mathbf{r})$ which has the periodicity of the crystal's Bravais lattice,

$$U(\mathbf{r} + \mathbf{R}) = U(\mathbf{r}), \qquad \forall\ \mathbf{R} \text{ in Bravais lattice.} \tag{A.36}$$

Consider the following Hamiltonian for electrons:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) \tag{A.37}$$

for which the Schrödinger equation reads

$$H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right)\psi = E\psi. \tag{A.38}$$

Bloch's theorem states that the one-electron wavefunctions can be chosen to have the form of a plane wave multiplied by a function having the periodicity of the Bravais lattice, *i.e.*

$$\boxed{\psi_{\mathbf{k}n}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}n}(\mathbf{r})} \tag{A.39}$$

in which n is a band index and

$$u_{\mathbf{k}n}(\mathbf{r} + \mathbf{R}) = u_{\mathbf{k}n}(\mathbf{r}) \qquad \forall\ \mathbf{R} \text{ in Bravais lattice.} \tag{A.40}$$

One consequence of Bloch's theorem is that the wavefunctions are quasi-periodic,

$$\psi_{\mathbf{k}n}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{\mathbf{k}n}(\mathbf{r}). \tag{A.41}$$

More details concerning Bloch's theorem, including its proof, can be found in *e.g.* Ashcroft & Mermin, Chapter 8.

Wannier states

Wannier states are simply the Fourier transforms of the Bloch states:

$$\psi_{\mathbf{R}n} \equiv \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in \mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{R}}\psi_{\mathbf{k}n}, \qquad \psi_{\mathbf{k}n} \equiv \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{\mathbf{R}n}. \tag{A.42}$$

The Wannier functions are peaked around the corresponding atomic site labelled by $\mathbf{R}$.

Exercises

TS Write the first two terms in the Taylor series around $x = x_0$ for a) e^x, b) x^α, c) $\ln x$.

Cauchy Perform the integral $\int_{-\infty}^{\infty} dx \frac{1}{x^2+a^2}$ using the residue theorem.

FT Let $f(x)$ be a periodic function with period L, $f(x+L) = f(x)$. What is the Fourier transform of $f^2(x)$? In other words, calculate $\int_0^L dx e^{-ik_n x} f^2(x)$ and express your answer in terms of the Fourier coefficients f_{k_n} of $f(x)$.

QHO. Show that the state $(\hat{a}^\dagger)^n|0\rangle$ is an eigenstate of the harmonic oscillator Hamiltonian. Normalize this state.

Answers to the exercises

$$e^{x_0+\epsilon} = e^{x_0}\sum_{n=0}^{\infty}\frac{1}{n!}\epsilon^n = 1+\epsilon+\frac{1}{2}\epsilon^2+....$$

$$(x_0+\epsilon)^\alpha = x_0^\alpha(1+\epsilon/x_0)^\alpha = x_0^\alpha(1+\alpha\epsilon/x_0+\frac{\alpha(\alpha-1)}{2}(\epsilon/x_0)^2+...).$$

$$\ln(x_0+\epsilon) = \ln x_0+\ln(1+\epsilon/x_0) = \ln x_0+\epsilon/x_0+\frac{1}{2}(\epsilon/x_0)^2+\frac{1}{3}(\epsilon/x_0)^3+... = \ln x_0+\sum_{n=1}^{\infty}\frac{1}{n}(\epsilon/x_0)^n$$

$$\int_{-\infty}^{\infty}dx\frac{1}{x^2+a^2} = \int_{-\infty}^{\infty}\frac{dx}{2ia}\left(\frac{1}{x-ia}-\frac{1}{x+ia}\right) = \frac{2\pi i}{2ia}Res_{1/(x-ia)}(ia) = \pi$$

by using a contour encircling the upper half-plane counterclockwise.

$$\int_0^L dxe^{-ik_nx}f^2(x) = \int_0^L dxe^{-ik_nx}\left(\frac{1}{L}\sum_{n_1}e^{ik_{n_1}x}f_{k_{n_1}}\right)\left(\frac{1}{L}\sum_{n_2}e^{ik_{n_2}x}f_{k_{n_2}}\right)$$

$$= \frac{1}{L^2}\sum_{n_1,n_2}f_{k_{n_1}}f_{k_{n_2}}\int_0^L dxe^{i(k_{n_1}+k_{n_2}-k_n)x} = \frac{1}{L}\sum_{n_1,n_2}f_{k_{n_1}}f_{k_{n_2}}\delta_{n_1+n_2,n} = \frac{1}{L}\sum_{n_1}f_{k_{n_1}}f_{k_{n-n_1}}.$$

By induction, one can prove that $[\hat{a},(\hat{a}^\dagger)^n] = n(\hat{a}^\dagger)^{n-1}$. Then,

$$\begin{aligned}H(\hat{a}^\dagger)^n|0\rangle = \hbar\omega(\hat{a}^\dagger\hat{a}+1/2)(\hat{a}^\dagger)^n|0\rangle &= \hbar\omega(\hat{a}^\dagger((\hat{a}^\dagger)^n\hat{a}+n(\hat{a}^\dagger)^{n-1})+\frac{1}{2}(\hat{a}^\dagger)^n)|0\rangle\\ &= \hbar\omega(n+\frac{1}{2})(\hat{a}^\dagger)^n|0\rangle\end{aligned}$$

so this is an eigenstate of energy $(n+\frac{1}{2})\hbar\omega$. Its square norm is

$$\begin{aligned}\langle 0|\hat{a}^n(\hat{a}^\dagger)^n|0\rangle = \langle 0|\hat{a}^{n-1}((\hat{a}^\dagger)^n a+n(\hat{a}^\dagger)^{n-1})|0\rangle &= n\langle 0|\hat{a}^{n-1}(\hat{a}^\dagger)^{n-1}|0\rangle\\ = n(n-1)\langle 0|\hat{a}^{n-2}(\hat{a}^\dagger)^{n-2}|0\rangle = ... = n!\langle 0|0\rangle &= n!\end{aligned}$$

so a properly normalized state is $\frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle$.

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