Lecture Notes for the C6 Theory Option

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Part I
Functional Methods in Quantum Mechanics

1 Some Mathematical Background

Functional Methods form a central part of modern theoretical physics. In the following we introduce the notion of functionals and how to manipulate them.

1.1 Functionals

What is a *functional*? You all know that a real function can be viewed as a *map* from e.g. an interval $[a, b]$ to the real numbers

$$f : [a, b] \to \mathbb{R} \ , \quad x \to f(x). \tag{1}$$

A functional is similar to a function in that it maps all elements in a certain domain to real numbers, however, the nature of its domain is very different. Instead of acting on all points of an interval or some other subset of the real numbers, the domain of functionals consists of (suitably chosen) classes of functions. In other words, given some class $\{f\}$ of functions, a functional F is a map

$$F : \{f\} \to \mathbb{R} \ , \quad f \to F[f]. \tag{2}$$

We now consider two specific examples of functionals.

1. The distance between two points. A very simple functional F consists of the map which assigns to all paths between two fixed points the length of the path. To write this functional explicitly, let us consider a simple two-dimensional situation in the (x, y) plane and choose two points (x_1, y_1) and (x_2, y_2). We consider the set of paths that do not turn back, i.e. paths along which x increases monotonically as we go from (x_1, y_1) to (x_2, y_2). These can be described by the set of functions $\{f\}$ on the interval $[x_1, x_2]$ satisfying $f(x_1) = y_1$ and $f(x_2) = y_2$. The length of a path is then given by the well-known expression

$$F[f(x)] = \int_{x_1}^{x_2} dx' \, \sqrt{1 + f'(x')^2} \ . \tag{3}$$

2. *Action Functionals.* These are very important in Physics. Let us recall their definition in the context of classical mechanics. Start with n generalised coordinates $\mathbf{q}(t) = (q_1(t), \ldots, q_n(t))$ and a Lagrangian $L = L(\mathbf{q}, \dot{\mathbf{q}})$. Then, the action functional $S[\mathbf{q}]$ is defined by

$$S[\mathbf{q}] = \int_{t_1}^{t_2} dt \, L(\mathbf{q}(t), \dot{\mathbf{q}}(t)) \ . \tag{4}$$

It depends on classical paths $\mathbf{q}(t)$ between times t_1 and t_2 satisfying the boundary conditions $\mathbf{q}(t_1) = \mathbf{q}_1$ and $\mathbf{q}(t_2) = \mathbf{q}_2$.

1.2 Functional differentiation

In both the examples given above a very natural question to ask is what function *extremizes* the functional. In the first example this corresponds to wanting to know the path that minimizes the distance between two points. In the second example the extremum of the action functional gives the solutions to the classical equations of motion. This is known as *Hamilton's principle*. In order to figure out what function extremizes the functional it is very useful to generalize the notion of a derivative. For our purposes we define the *functional derivative* by

$$\boxed{\frac{\delta F[f(x)]}{\delta f(y)} = \lim_{\epsilon\to 0} \frac{F[f(x)+\epsilon\delta(x-y)] - F[f(x)]}{\epsilon}} \ . \tag{5}$$

Here, as usual, we should think of the δ-function as being defined as the limit of a test function, e.g.

$$\delta(x) = \lim_{a\to 0} \frac{1}{\sqrt{\pi}a} e^{-x^2/a^2} \ , \tag{6}$$

and take the limit $a \to 0$ only in the end (after commuting the limit with all other operations such as the $\lim_{\epsilon\to 0}$ in (5)). Importantly, the derivative defined in this way is a linear operation which satisfies the product and chain rules of ordinary differentiation and commutes with ordinary integrals and derivatives. Let us see how functional differentiation works for our two examples.

1. The distance between two points. In analogy with finding stationary points of functions we want to extremize (3) by setting its functional derivative equal to zero

$$0 = \frac{\delta F[f(x)]}{\delta f(y)} \ . \tag{7}$$

We first do the calculation by using the definition (5).

$$\frac{\delta F[f(x)]}{\delta f(y)} = \lim_{\epsilon\to 0} \int_{x_1}^{x_2} dx' \ \frac{\sqrt{1+\left[f'(x')+\epsilon\delta'(x'-y)\right]^2} - \sqrt{1+\left[f'(x')\right]^2}}{\epsilon}. \tag{8}$$

The Taylor expansion of the square root is $\sqrt{1+2\epsilon} = 1+\epsilon+\ldots$, which gives

$$\sqrt{1+\left[f'(x')+\epsilon\delta'(x'-y)\right]^2} \ = \ \sqrt{1+\left[f'(x')\right]^2} + \frac{\epsilon f'(x')\delta'(x'-y)}{\sqrt{1+\left[f'(x')\right]^2}} + \mathcal{O}(\epsilon^2) \ , \tag{9}$$

where $\delta'(x)$ is the derivative of the delta-function and $\mathcal{O}(\epsilon^2)$ denote terms proportional to ϵ^2. Substituting this back into (8) we have [1]

$$\frac{\delta F[f(x)]}{\delta f(y)} = \int_{x_1}^{x_2} dx' \ \frac{\delta'(x'-y)f'(x')}{\sqrt{1+\left[f'(x')\right]^2}} = -\frac{d}{dy}\frac{f'(y)}{\sqrt{1+\left[f'(y)\right]^2}}. \tag{11}$$

The solution to (7) is thus

$$f'(y) = \text{const}, \tag{12}$$

which describes a straight line. In practice we don't really go back to the definition of the functional derivative any more than we use the definition of an ordinary derivative to work it out, but proceed as follows.

[1] In the last step we have used

$$\int_a^b dx'\delta'(x'-y)g(x') = -g'(y) \ , \tag{10}$$

which can be proved by "integration by parts".

- We first interchange the functional derivative and the integration

$$\frac{\delta F[f(x)]}{\delta f(y)} = \int_{x_1}^{x_2} dx' \; \frac{\delta}{\delta f(y)} \sqrt{1 + [f'(x')]^2}. \tag{13}$$

- Next we use the chain rule

$$\frac{\delta \sqrt{1+f'(x')^2}}{\delta f(y)} = \frac{1}{2\sqrt{1+f'(x')^2}} \frac{\delta(1+f'(x')^2)}{\delta f(y)} = \frac{f'(x')}{\sqrt{1+f'(x')^2}} \frac{\delta f'(x')}{\delta f(y)}. \tag{14}$$

- Finally we interchange the functional and the ordinary derivative

$$\frac{\delta f'(x')}{\delta f(y)} = \frac{d}{dx'} \frac{\delta f(x')}{\delta f(y)} = \frac{d}{dx'} \delta(x'-y) \; . \tag{15}$$

  The last identity follows from our definition (5).

Now we can put everything together and arrive at the same answer (11).

EXERCISE

2. Next we want to try out these ideas on our second example and extremize the classical action (4) in order to obtain the classical equations of motion. We first interchange functional derivative and integration and then use the chain rule to obtain

$$\begin{aligned} \frac{\delta S[\mathbf{q}]}{\delta q_i(t)} &= \frac{\delta}{\delta q_i(t)} \int_{t_1}^{t_2} d\tilde{t} \, L(\mathbf{q}(\tilde{t}), \dot{\mathbf{q}}(\tilde{t})) & (16) \\ &= \int_{t_1}^{t_2} d\tilde{t} \left[\frac{\partial L}{\partial q_j}(\mathbf{q}, \dot{\mathbf{q}}) \frac{\delta q_j(\tilde{t})}{\delta q_i(t)} + \frac{\partial L}{\partial \dot{q}_j}(\mathbf{q}, \dot{\mathbf{q}}) \frac{\delta \dot{q}_j(\tilde{t})}{\delta q_i(t)} \right] & (17) \\ & & (18) \end{aligned}$$

We now use that $\frac{\delta \dot{q}_j(\tilde{t})}{\delta q_i(t)} = \frac{d}{d\tilde{t}} \frac{\delta q_j(\tilde{t})}{\delta q_i(t)}$ and integrate by parts with respect to $\tilde{t}$

$$\begin{aligned} \frac{\delta S[\mathbf{q}]}{\delta q_i(t)} &= \int_{t_1}^{t_2} d\tilde{t} \left[\frac{\partial L}{\partial q_j}(\mathbf{q}, \dot{\mathbf{q}}) - \frac{d}{d\tilde{t}} \frac{\partial L}{\partial \dot{q}_j}(\mathbf{q}, \dot{\mathbf{q}}) \right] \frac{\delta q_j(\tilde{t})}{\delta q_i(t)} & (19) \\ &= \int_{t_1}^{t_2} d\tilde{t} \left[\frac{\partial L}{\partial q_j}(\mathbf{q}, \dot{\mathbf{q}}) - \frac{d}{d\tilde{t}} \frac{\partial L}{\partial \dot{q}_j}(\mathbf{q}, \dot{\mathbf{q}}) \right] \delta_{ij} \delta(\tilde{t} - t) = \frac{\partial L}{\partial q_i}(\mathbf{q}, \dot{\mathbf{q}}) - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i}(\mathbf{q}, \dot{\mathbf{q}}) \; . & (20) \end{aligned}$$

In the second last step we have used

$$\frac{\delta q_j(\tilde{t})}{\delta q_i(t)} = \delta_{ij} \delta(\tilde{t} - t) \; , \tag{21}$$

which follows straightforwardly from our general definition (5). Thus we conclude that the extrema of the classical action are given by paths that fulfil the equations of motion

$$\boxed{\frac{\partial L}{\partial q_i}(\mathbf{q}, \dot{\mathbf{q}}) - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i}(\mathbf{q}, \dot{\mathbf{q}}) = 0.} \tag{22}$$

Nice.

EXERCISE

1.3 Multidimensional Gaussian Integrals

As a reminder, we start with a simple one-dimensional Gaussian integral over a single variable y. It is given by

$$\boxed{I(z) \equiv \int_{-\infty}^{\infty} dy\, \exp(-\frac{1}{2}zy^2) = \sqrt{\frac{2\pi}{z}}\,,} \tag{23}$$

where z is a complex number with $\mathrm{Re}(z) > 0$. The standard proof of this relation involves writing $I(z)^2$ as a two-dimensional integral over y_1 and y_2 and then introducing two-dimensional polar coordinates $r = \sqrt{y_1^2 + y_2^2}$ and φ. Explicitly,

$$I(z)^2 = \int_{-\infty}^{\infty} dy_1\, \exp(-\frac{1}{2}zy_1^2) \int_{-\infty}^{\infty} dy_2\, \exp(-\frac{1}{2}zy_2^2) = \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2\, \exp(-\frac{1}{2}z(y_1^2+y_2^2)) \tag{24}$$

$$= \int_0^{2\pi} d\varphi \int_0^{\infty} dr\, r \exp(-\frac{1}{2}zr^2) = \frac{2\pi}{z}\,. \tag{25}$$

Next we consider n-dimensional Gaussian integrals

$$W_0(\mathbf{A}) \equiv \int d^n\mathbf{y}\, \exp\left(-\frac{1}{2}\mathbf{y}^T\mathbf{A}\mathbf{y}\right)\,, \tag{26}$$

over variables $\mathbf{y} = (y_1, \ldots, y_n)$, where $\mathbf{A}$ is a symmetric, positive definite matrix (all its eigenvalues are positive). This integral can be reduced to a product of one-dimensional Gaussian integrals by diagonalising the matrix $\mathbf{A}$. Consider an orthogonal rotation $\mathbf{O}$ such that $\mathbf{A} = \mathbf{O}\mathbf{D}\mathbf{O}^T$ with a diagonal matrix $\mathbf{D} = \mathrm{diag}(a_1, \ldots, a_n)$. The eigenvalues a_i are strictly positive since we have assumed that $\mathbf{A}$ is positive definite. Introducing new coordinates $\tilde{\mathbf{y}} = \mathbf{O}^T\mathbf{y}$ we can write

$$\mathbf{y}^T\mathbf{A}\mathbf{y} = \tilde{\mathbf{y}}^T\mathbf{D}\tilde{\mathbf{y}} = \sum_{i=1}^{n} a_i\tilde{y}_i^2\,, \tag{27}$$

where the property $\mathbf{O}^T\mathbf{O} = \mathbf{1}$ of orthogonal matrices has been used. Note further that the Jacobian of the coordinate change $\mathbf{y} \to \tilde{\mathbf{y}}$ is one, since $|\det(\mathbf{O})| = 1$. Hence, using Eqs. (23) and (27) we find for the integral (26)

$$W_0(\mathbf{A}) = \prod_{i=1}^{n} \int d\tilde{y}_i \exp(-\frac{1}{2}a_i\tilde{y}_i^2) = (2\pi)^{n/2}(a_1a_2\ldots a_n)^{-1/2} = (2\pi)^{n/2}(\det\mathbf{A})^{-1/2}\,. \tag{28}$$

To summarise, we have found for the multidimensional Gaussian integral (26) that

$$\boxed{W_0(\mathbf{A}) = (2\pi)^{n/2}(\det\mathbf{A})^{-1/2}\,,} \tag{29}$$

a result which will be of some importance in the following. We note that if we multiply the matrix $\mathbf{A}$ by a complex number z with $\mathrm{Re}(z) > 0$ and then follow through exactly the same steps, we find

$$W_0(z\mathbf{A}) = \left(\frac{2\pi}{z}\right)^{n/2} (\det\mathbf{A})^{-1/2}\,. \tag{30}$$

One obvious generalisation of the integral (26) involves adding a term linear in $\mathbf{y}$ in the exponent, that is

$$W_0(\mathbf{A}, \mathbf{J}) \equiv \int d^n\mathbf{y}\, \exp\left(-\frac{1}{2}\mathbf{y}^T\mathbf{A}\mathbf{y} + \mathbf{J}^T\mathbf{y}\right)\,. \tag{31}$$

Here $\mathbf{J} = (J_1, \ldots, J_n)$ is an n-dimensional vector. Changing variables $\mathbf{y} \to \tilde{\mathbf{y}}$, where

$$\mathbf{y} = \mathbf{A}^{-1}\mathbf{J} + \tilde{\mathbf{y}} \tag{32}$$

this integral can be written as

$$W_0(\mathbf{A}, \mathbf{J}) = \exp\left(\frac{1}{2}\mathbf{J}^T\mathbf{A}^{-1}\mathbf{J}\right) \int d^n\tilde{\mathbf{y}}\, \exp\left(-\frac{1}{2}\tilde{\mathbf{y}}^T\mathbf{A}\tilde{\mathbf{y}}\right) . \tag{33}$$

The remaining integral is Gaussian without a linear term, so can be easily carried out using the above results. Hence, one finds

$$\boxed{W_0(\mathbf{A}, \mathbf{J}) = (2\pi)^{n/2}(\det\mathbf{A})^{-1/2} \exp\left(\frac{1}{2}\mathbf{J}^T\mathbf{A}^{-1}\mathbf{J}\right) .} \tag{34}$$

1.4 Homework Questions 1&2

Question 1. Consider paths $\mathbf{X} = \mathbf{X}(\tau)$, where τ is a parameter, and the functional

$$l[\mathbf{X}] = \int_{\tau_0}^{\tau_1} d\tau\, n(\mathbf{X}) \sqrt{\frac{d\mathbf{X}}{d\tau} \cdot \frac{d\mathbf{X}}{d\tau}} ,$$

where $n = n(\mathbf{X})$ is a function. (The minima of this functional can be interpreted as light rays propagating in a medium with refractive index n.)
a) Derive the differential equation which has to be satisfied by minimal paths $\mathbf{X}$.
b) Consider a two-dimensional situation with paths $\mathbf{X}(\tau) = (X(\tau), Y(\tau))$ in the x, y plane and a function $n = n_0 + (n_1 - n_0)\,\theta(x)$. (The Heaviside function $\theta(x)$ is defined to be 0 for $x < 0$ and 1 for $x \geq 0$. Recall that $\theta'(x) = \delta(x)$.) Solve the differential equation in a) for this situation, using the coordinate x as parameter τ along the path.
c) Show that the solution in b) leads to the standard law for refraction at the boundary between two media with refractive indices n_0 and n_1.

Question 2. a) Evaluate the Gaussian integral

$$\int_{-\infty}^{\infty} dx\; e^{-\frac{1}{2}zx^2} \tag{35}$$

for a complex constant z. What is the requirement on z for the integral to exist?
b) The gamma function Γ is defined by

$$\Gamma(s+1) = \int_0^{\infty} dx\, x^s e^{-x} .$$

c) Show that $\Gamma(1) = 1$ and $\Gamma(s+1) = s\Gamma(s)$. (Hence $\Gamma(n+1) = n!$)
d) Take s to be real and positive. Evaluate $\Gamma(s+1)$ in the *steepest descent approximation*: write the integrand in the form $e^{f(x)}$ and argue that for large $s \gg 1$ the dominant contribution to the integral arises from the minima of $f(x)$. Expand the function to quadratic order around the minimum, argue that you may extend the integration boundaries to $\pm\infty$, and then carry out the resulting integral. Your result is known as *Stirling's approximation*: it tells you what $n!$ is when n becomes large.
e)* The following extension is for complex analysis afficionados, so simply omit it if you haven't taken the short option. Take s to be complex with positive real part. Deform the contour in a suitable way, so that you can again apply a steepest descent approximation. Ponder the name of the method. What is Stirling's approximation for complex s?

2 Path Integrals in Quantum Mechanics

So far you have encountered two ways of doing QM:

1. Following Schrödinger, we can solve the Schrödinger equation for the wave function → Fun with PDEs...

2. Following Heisenberg, we can work with operators, commutation relations, eigenstates → Fun with Linear Algebra...

Historically it took some time for people to realize that these are in fact equivalent. To quote the great men: *I knew of Heisenberg's theory, of course, but I felt discouraged, not to say repelled, by the methods of transcendental algebra, which appeared difficult to me, and by the lack of visualizability. (Schrödinger in 1926)*

The more I think about the physical portion of Schrödinger's theory, the more repulsive I find it. What Schrödinger writes about the visualizability of his theory is probably not quite right, in other words it's crap. (Heisenberg, writing to Pauli in 1926)

There is a third approach to QM, due to *Feynman*. He developed it when he was a graduate student, inspired by a mysterious remark in a paper by Dirac. Those were the days! Feynman's approach is particularly useful for QFTs and many-particle QM problems, as it makes certain calculations much easier. We will now introduce it by working backwards. The central object in Feynman's method is something called a *propagator*. We'll now work out what this is using the Heisenberg/Schrödinger formulation of QM you know and love. After we have done that, we formulate QM à la Feynman.

2.1 The Propagator

Our starting point is the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle. \tag{36}$$

We recall that the wave function is given by

$$\psi(\vec{x},t) = \langle\vec{x}|\psi(t)\rangle. \tag{37}$$

Eqn (36) can be integrated to give

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi(0)\rangle \tag{38}$$

The *time-evolution operator* in QM is thus (assuming that H is time-independent)

$$U(t;t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}. \tag{39}$$

A central object in Feynman's approach is the *propagator*

$$\boxed{\langle\vec{x}'|U(t;t_0)|\vec{x}\rangle,} \tag{40}$$

where $|\vec{x}\rangle$ are the simultaneous eigenstates of the position operators $\hat{x}$, $\hat{y}$ and $\hat{z}$. The propagator is the probability amplitude for finding our QM particle at position $\vec{x}'$ at time t, if it started at position $\vec{x}$ at time t_0. To keep notations simple, we now consider a particle moving in one dimension with time-independent Hamiltonian

$$H = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + V(\hat{x}). \tag{41}$$

We want to calculate the propagator

$$\langle x_N|U(t;0)|x_0\rangle. \tag{42}$$

It is useful to introduce small time steps

$$t_n = n\epsilon \ , \quad n = 0, \ldots, N, \tag{43}$$

where $\epsilon = t/N$. Then we have by construction

$$U(t;0) = \left(e^{-\frac{i}{\hbar}H\epsilon}\right)^N . \tag{44}$$

The propagator is

$$\begin{aligned} \langle x_N|U(t;0)|x_0\rangle &= \langle x_N|e^{-\frac{i}{\hbar}H\epsilon}\cdots e^{-\frac{i}{\hbar}H\epsilon}|x_0\rangle \\ &= \int dx_{N-1}\ldots\int dx_1\ \langle x_N|e^{-\frac{i}{\hbar}H\epsilon}|x_{N-1}\rangle\langle x_{N-1}|e^{-\frac{i}{\hbar}H\epsilon}|x_{N-2}\rangle\ldots\langle x_1|e^{-\frac{i}{\hbar}H\epsilon}|x_0\rangle, \end{aligned} \tag{45}$$

where we have inserted $N-1$ resolutions of the identity in terms of position eigenstates

$$\mathbf{1} = \int dx\ |x\rangle\langle x| \ . \tag{46}$$

This expression now has a very nice and intuitive interpretation, see Fig. 1: The propagator, i.e. the

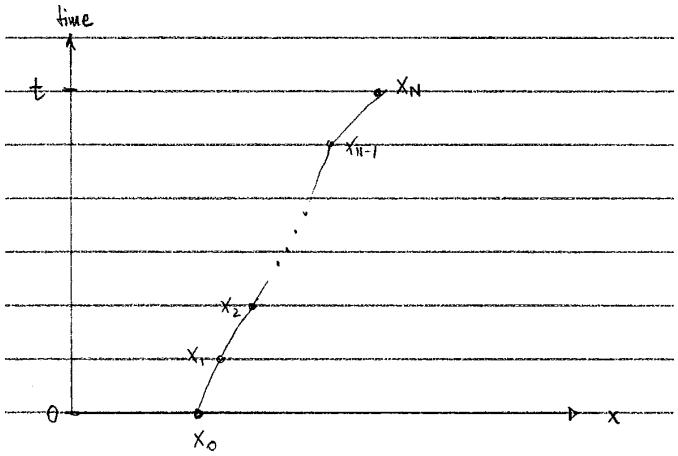


Figure 1: Propagator as sum over paths.

probabilty amplitude for finding the particle at position x_N and time t given that it was at position x_0 at time 0 is given by the sum over all "paths" going from x_0 to x_N (as $x_1,\ldots,\ x_{N-1}$ are integrated over).

In the next step we determine the "infinitesimal propagator"

$$\langle x_{n+1}|e^{-\frac{i}{\hbar}H\epsilon}|x_n\rangle. \tag{47}$$

Importantly we have $[\hat{T},\hat{V}] \neq 0$ and concomitantly

$$e^{\alpha(\hat{T}+\hat{V})} \neq e^{\alpha\hat{T}}e^{\alpha\hat{V}}. \tag{48}$$

However, using that ϵ is infinitesimal, we have

$$\begin{aligned} e^{-\frac{i}{\hbar}\epsilon(\hat{T}+\hat{V})} &= 1 - \frac{i}{\hbar}\epsilon(\hat{T}+\hat{V}) + \mathcal{O}(\epsilon^2) \ , \\ e^{-\frac{i}{\hbar}\epsilon\hat{T}}e^{-\frac{i}{\hbar}\epsilon\hat{V}} &= 1 - \frac{i}{\hbar}\epsilon(\hat{T}+\hat{V}) + \mathcal{O}(\epsilon^2). \end{aligned} \tag{49}$$

So up to terms of order ϵ^2 we have

$$\langle x_{n+1}|e^{-\frac{i}{\hbar}H\epsilon}|x_n\rangle \simeq \langle x_{n+1}|e^{-\frac{i}{\hbar}\hat{T}\epsilon}e^{-\frac{i}{\hbar}\hat{V}\epsilon}|x_n\rangle = \langle x_{n+1}|e^{-\frac{i}{\hbar}\hat{T}\epsilon}|x_n\rangle e^{-\frac{i}{\hbar}V(x_n)\epsilon}, \tag{50}$$

where we have used that $\hat{V}|x\rangle = V(x)|x\rangle$. As $\hat{T} = \hat{p}^2/2m$ it is useful to insert a complete set of momentum eigenstates [2] to calculate

$$\begin{aligned}\langle x_{n+1}|e^{-\frac{i}{\hbar}\hat{T}\epsilon}|x_n\rangle &= \int \frac{dp}{2\pi\hbar}\langle x_{n+1}|e^{-\frac{i\hat{p}^2\epsilon}{2m\hbar}}|p\rangle\langle p|x_n\rangle = \int \frac{dp}{2\pi\hbar}e^{-\frac{ip^2\epsilon}{2m\hbar}-i\frac{p}{\hbar}(x_n-x_{n+1})} \\ &= \sqrt{\frac{m}{2\pi i\hbar\epsilon}}e^{\frac{im}{2\hbar\epsilon}(x_n-x_{n+1})^2}. \end{aligned} \tag{51}$$

In the second step we have used that $\hat{p}|p\rangle = p|p\rangle$ and that

$$\langle x|p\rangle = e^{\frac{ipx}{\hbar}}. \tag{52}$$

The integral over p is performed by changing variables to $p' = p + \frac{m}{\epsilon}(x_n - x_{n+1})$ (and giving ϵ a very small imaginary part in order to make the integral convergent). Substituting (51) and (50) back into our expression (45) for the propagator gives

$$\boxed{\langle x_N|U(t;0)|x_0\rangle = \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}}\int dx_1\ldots dx_{N-1}\exp\left(\frac{i\epsilon}{\hbar}\sum_{n=0}^{N-1}\frac{m}{2}\left(\frac{x_{n+1}-x_n}{\epsilon}\right)^2 - V(x_n)\right)} \tag{53}$$

Note that in this expression there are no operators left.

2.1.1 Propagator as a "Functional Integral"

The way to think about (53) is as a *sum over trajectories*:

- $x_0, \ldots, x_N$ constitute a discretization of a *path* $x(t')$, where we set $x_n \equiv x(t_n)$.
- We then have
$$\frac{x_{n+1}-x_n}{\epsilon} = \frac{x(t_{n+1})-x(t_n)}{t_{n+1}-t_n} \simeq \dot{x}(t_n), \tag{54}$$
and
$$\epsilon\sum_{n=0}^{N-1}\frac{m}{2}\left(\frac{x_{n+1}-x_n}{\epsilon}\right)^2 - V(x_n) \simeq \int_0^t dt'\left[\frac{m}{2}\dot{x}^2(t') - V(x)\right] \equiv \int_0^t dt'\mathcal{L}[\dot{x},x], \tag{55}$$
where $\mathcal{L}$ is the *Lagrangian* of the system. In classical mechanics the time-integral of the Lagrangian is known as the *action*
$$S = \int_0^t dt'\mathcal{L}. \tag{56}$$
- The integral over $x_1, \ldots x_{N-1}$ becomes a *functional integral*, also known as a *path integral*, over all paths $x(t')$ that start at x_0 at time $t' = 0$ and end at x_N at time $t' = t$.
- The prefactor in (53) gives rise to an overall (infinite) normalization and we will denote it by $\mathcal{N}$.

These considerations lead us to express the propagator as the following *formal expression*

$$\boxed{\langle x_N|U(t;0)|x_0\rangle = \mathcal{N}\int\mathcal{D}x(t')\; e^{\frac{i}{\hbar}S[x(t')]}.} \tag{57}$$

What is in fact meant by (57) is the limit of the discretized expression (53). The ultimate utility of (57) is that it provides a compact notation, that on the one hand will allow us to manipulate functional integrals, and on the other hand provides a nice, intuitive interpretation.

[2] We use a normalization $\langle p|k\rangle = 2\pi\hbar\delta(p-k)$, so that $\mathbf{1} = \int\frac{dp}{2\pi\hbar}|p\rangle\langle p|$.

2.2 Quantum Mechanics à la Feynman

Feynman's formulation of Quantum Mechanics is based on the single postulate that the probability amplitude for propagation from a position x_0 to a position x_N is obtained by summing over all possible paths connecting x_0 and x_N, where each path is *weighted* by a phase factor $\exp\left(\frac{i}{\hbar}S\right)$, where S is the *classical action* of the path. This provides a new way of thinking about QM!

2.3 Classical Limit and Stationary Phase Approximation

An important feature of (57) is that it gives us a nice way of thinking about the classical limit "$\hbar \to 0$" (more precisely in the limit when the dimensions, masses, times etc are so large that the action is huge compared to $\hbar$). To see what happens in this limit let us first consider the simpler case of an ordinary integral

$$g(a) = \int_{-\infty}^{\infty} dt\ h_1(t) e^{iah_2(t)}, \tag{58}$$

when we take the real parameter a to infinity. In this case the integrand will oscillate wildly as a function of t because the phase of $\exp\left(iah_2(t)\right)$ will vary rapidly. The dominant contribution will arise from the points where the phase changes slowly, which are the stationary points

$$h_2'(t) = 0. \tag{59}$$

The integral can then be approximated by expanding around the stationary points. Assuming that there is a single stationary point at t_0

$$g(a \gg 1) \approx \int_{-\infty}^{\infty} dt \left[h_1(t_0) + (t-t_0)h_1'(t_0) + \ldots\right] e^{iah_2(t_0) + i\frac{ah_2''(t_0)}{2}(t-t_0)^2}, \tag{60}$$

Changing integration variables to $t' = t - t_0$ (and giving a a small imaginary part to make the integral converge at infinity) as obtain a Gaussian integral that we can take using (23)

$$g(a \gg 1) \approx \sqrt{\frac{2\pi i}{ah_2''(t_0)}} h_1(t_0) e^{iah_2(t_0)}\ . \tag{61}$$

Subleading contributions can be evaluated by taking higher order contributions in the Taylor expansions into account. If we have several stationary points we sum over their contributions. The method we have just discussed is known as *stationary phase approximation*.

The generalization to path integrals is now clear: in the limit $\hbar \to 0$ the path integral is dominated by the vicinity of the *stationary points* of the action S

$$\frac{\delta S}{\delta x(t')} = 0. \tag{62}$$

The condition (62) precisely defines the *classical trajectories* $x(t')$!

2.4 The Propagator for Free Particles

We now wish to calculate the functional integral (57) for a free particle, i.e.

$$V(x) = 0. \tag{63}$$

Going back to the explicit expression (53) we have

$$\langle x_N|U(t;0)|x_0\rangle \;=\; \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}} \int dx_1 \ldots dx_{N-1} \exp\left(\frac{i\epsilon}{\hbar}\sum_{n=0}^{N-1}\frac{m}{2}\left(\frac{x_{n+1}-x_n}{\epsilon}\right)^2\right)\ . \tag{64}$$

It is useful to change integration variables to

$$y_j = x_j - x_N \ , \quad j = 1, \ldots, N-1, \tag{65}$$

which leads to an expression

$$\langle x_N|U(t;0)|x_0\rangle \ = \ \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}} \int d\mathbf{y}\exp\left(-\frac{1}{2}\mathbf{y}^T\mathbf{A}\mathbf{y} + \mathbf{J}^T\cdot\mathbf{y}\right) e^{\frac{im}{2\hbar\epsilon}(x_0-x_N)^2}. \tag{66}$$

Here

$$\mathbf{J}^T = \left(\frac{im}{\hbar\epsilon}(x_N - x_0), 0, \ldots, 0\right), \tag{67}$$

and $\mathbf{A}$ is a $(N-1)\times(N-1)$ matrix with elements

$$A_{jk} = \frac{-im}{\epsilon\hbar}\left[2\delta_{j,k} - \delta_{j,k+1} - \delta_{j,k-1}\right]. \tag{68}$$

For a given N (66) is a multidimensional Gaussian integral and can be carried out using (34)

$$\langle x_N|U(t;0)|x_0\rangle \ = \ \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}} (2\pi)^{\frac{N-1}{2}}\left[\det(\mathbf{A})\right]^{-\frac{1}{2}}\exp\left(\frac{1}{2}\mathbf{J}^T\mathbf{A}^{-1}\mathbf{J}\right) e^{\frac{im}{2\hbar\epsilon}(x_0-x_N)^2}. \tag{69}$$

The matrix $\mathbf{A}$ is related to the one dimensional lattice Laplacian, see below. Given the eigenvalues and eigenvectors worked out below we can calculate the determinant and inverse of $\mathbf{A}$ (homework problem). Substituting the results into (69) gives

$$\boxed{\langle x_N|U(t;0)|x_0\rangle = \sqrt{\tfrac{m}{2\pi i\hbar t}}\, e^{\frac{im}{2\hbar t}(x_0-x_N)^2}.} \tag{70}$$

For a free particle we can evaluate the propagator directly in a much simpler way.

$$\begin{aligned}\langle x_N|U(t;0)|x_0\rangle \ &= \ \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\langle x_N|e^{-i\frac{\hat{p}^2 t}{2m\hbar}}|p\rangle\langle p|x_0\rangle = \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}e^{-i\frac{p^2 t}{2m\hbar}-i\frac{p(x_0-x_N)}{\hbar}} \\ &= \ \sqrt{\frac{m}{2\pi i\hbar t}}\, e^{\frac{im}{2\hbar t}(x_0-x_N)^2}.\end{aligned} \tag{71}$$

Aside: Lattice Laplacian

The matrix A is related to the one dimensional *Lattice Laplacian*. Consider functions of a variable $z_0 \le z \le z_N$ with "hard-wall boundary conditions"

$$f(z_0) = f(z_N) = 0. \tag{72}$$

The Laplace operator D acts on these functions as

$$Df \equiv \frac{d^2 f(z)}{dz^2}. \tag{73}$$

Discretizing the variable z by introducing $N-1$ points

$$z_n = z_0 + na_0 \ , \quad n = 1, \ldots, N-1 \tag{74}$$

where $a_0 = (z_N - z_0)/N$ is a "lattice spacing", maps the function $f(z)$ to a $N-1$ dimensional vector

$$f(z) \to \mathbf{f} = (f(z_1), \ldots, f(z_{N-1})). \tag{75}$$

Recalling that

$$\frac{d^2 f}{dz^2}(z) = \lim_{a_0\to 0}\frac{f(z+a_0) + f(z-a_0) - 2f(z)}{a_0^2} \ , \tag{76}$$

we conclude that the Lapacian is discretized as follows

$$Df \to a_0^{-2}\mathbf{\Delta f}\ , \tag{77}$$

where

$$\Delta_{jk} = \delta_{j,k+1} + \delta_{j,k-1} - 2\delta_{j,k}. \tag{78}$$

Our matrix $\mathbf{A}$ is equal to $\frac{im}{\epsilon\hbar}\mathbf{\Delta}$. The eigenvalue equation

$$\mathbf{\Delta a}_n = \lambda_n \mathbf{a}_n, \quad n = 1, \ldots, N-1 \tag{79}$$

gives rise to a recurrence relation for the components $\mathbf{a}_{n,j}$ of $\mathbf{a}_n$

$$a_{n,j+1} + a_{n,j-1} - (2+\lambda_n)a_{n,j} = 0. \tag{80}$$

The boundary conditions $a_{n,N} = a_{n,0} = 0$ suggest the ansatz

$$a_{n,j} = C_n \sin\left(\frac{\pi n j}{N}\right). \tag{81}$$

Substituting this in to (80) gives

$$\lambda_n = 2\cos\left(\frac{\pi n}{N}\right) - 2\ , \quad n = 1, \ldots, N-1. \tag{82}$$

The normalized eigenvectors of $\mathbf{\Delta}$ are

$$\mathbf{a}_n = \frac{1}{\sqrt{\sum_{j=1}^{N-1}\sin^2\left(\frac{\pi n j}{N}\right)}}\begin{pmatrix}\sin\left(\frac{\pi n}{N}\right)\\ \sin\left(\frac{2\pi n}{N}\right)\\ \vdots \\ \sin\left(\frac{\pi(N-1)n}{N}\right).\end{pmatrix} = \sqrt{\frac{2}{N}}\begin{pmatrix}\sin\left(\frac{\pi n}{N}\right)\\ \sin\left(\frac{2\pi n}{N}\right)\\ \vdots \\ \sin\left(\frac{\pi(N-1)n}{N}\right).\end{pmatrix} \tag{83}$$

ASIDE: LATTICE LAPLACIAN

2.5 Homework Questions 3-5

Question 3. Consider a free quantum mechanical particle moving in one dimension. The Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\ . \tag{84}$$

We have shown in the lecture that the propagator can be represented in the form

$$\langle x_N|e^{-\frac{i}{\hbar}tH}|x_0\rangle \ = \ \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}}\int dx_1\ldots dx_{N-1}\exp\left(\frac{i\epsilon}{\hbar}\sum_{n=0}^{N-1}\frac{m}{2}\left(\frac{x_{n+1}-x_n}{\epsilon}\right)^2\right)\ . \tag{85}$$

a) Change variables from x_j to $y_j = x_j - x_N$ to bring it to the form

$$\langle x_N|e^{-\frac{i}{\hbar}tH}|x_0\rangle \ = \ \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}}\int d\mathbf{y}\exp\left(-\frac{1}{2}\mathbf{y}^T\mathbf{A}\mathbf{y} + \mathbf{J}^T\cdot\mathbf{y}\right)e^{\frac{im}{2\hbar\epsilon}(x_0-x_N)^2}. \tag{86}$$

Give expressions for $\mathbf{J}$ and $\mathbf{A}$.
b) Carry out the integrals over y_j to get an expression for the propagator in terms of $\mathbf{A}$ and $\mathbf{J}$.
c) Work out the eigenvalues λ_n and eigenvectors $\mathbf{a}_n$ of the matrix $\mathbf{A}$. You may find helpful hints in the lecture notes.
d) What is $\det(\mathbf{A})$? A useful identity you may use is

$$\prod_{j=1}^{N-1} 2\sin(\pi j/2N) = \sqrt{N}. \tag{87}$$

Now work out $\mathbf{J}^T\mathbf{A}^{-1}\mathbf{J}$ by working in the eigenbasis of $\mathbf{A}^{-1}$ (Hint: write this as $\mathbf{J}^T\mathbf{A}^{-1}\mathbf{J} = \mathbf{J}^T\mathbf{O}^T\mathbf{O}\mathbf{A}^{-1}\mathbf{O}^T\mathbf{O}\mathbf{J}$, where $\mathbf{O}^T\mathbf{O} = 1$ and $\mathbf{O}\mathbf{A}^{-1}\mathbf{O}^T$ is a diagonal matrix you have already calculated above.). A useful identity you may use is

$$\sum_{j=1}^{N-1} \cos^2(\pi j/2N) = \frac{N-1}{2}. \tag{88}$$

e) Use the result you have obtained to write an explicit expression for the propagator.

Question 4. Denote the propagator by

$$K(t,x;t'x') = \langle x|e^{-\frac{i}{\hbar}H(t-t')}|x'\rangle. \tag{89}$$

Show that the wave function $\psi(t,x) = \langle x|\Psi(t)\rangle$, where $|\Psi(t)\rangle$ is a solution to the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle, \tag{90}$$

fulfils the integral equation

$$\psi(t,x) = \int_{-\infty}^{\infty} dx'\ K(t,x;t'x')\ \psi(t',x'). \tag{91}$$

Question 5. Diffraction through a slit. A free particle starting at $x = 0$ when $t = 0$ is determined to pass between $x_0 - b$ and $x_0 + b$ at time T. We wish to calculate the probabilty of finding the particle at position x at time $t = T + \tau$.
a) Argue on the basis of Qu 5. that the (un-normalized) wave function can be written in the form

$$\psi(T+\tau,x) = \int_{-b}^{b} dy\ K(T+\tau,x;T,x_0+y)\ K(T,x_0+y;0,0)\ , \tag{92}$$

where

$$K(t,x;t'x') = \langle x|e^{-\frac{i}{\hbar}H(t-t')}|x'\rangle. \tag{93}$$

b) Using that the propagation for $0 \le t < T$ and $T \le t < T+\tau$ is that of a free particle, obtain an explicit integral representation for the wave function.
c) Show that the wave function can be expressed in terms of the *Fresnel integrals*

$$C(x) = \int_0^x dy\ \cos(\pi y^2/2)\ , \quad S(x) = \int_0^x dy\ \sin(\pi y^2/2)\ . \tag{94}$$

Hint: make a substitution $z = \alpha y + \beta$ with suitably chosen α and β.

Derive an expression for the ratio $P(T+\tau,x)/P(T+\tau,x_0)$, where $P(T+\tau,x)dx$ is the probability of finding the particle in the interval $[x, x+dx]$ at time $T+\tau$.
d)* If you can get hold of *Mathematica* (the default assumption is that you will not), plot the result as a function of the dimensionless parameter $x/[b(1+\tau/T)]$ for $x_0 = 0$ and different values of the ratio

$$\gamma = \frac{mb^2(1+\tau/T)}{\hbar\tau}\ . \tag{95}$$

Discuss your findings.

3 Path Integrals in Quantum Statistical Mechanics

Path integrals can also be used to describe quantum systems at finite temperatures. To see how this works we now consider a quantum mechanical particle coupled to a heat bath at a temperature T. An important quantity in Statistical Mechanics is the *partition function*

$$Z(\beta) = \mathrm{Tr}\left[e^{-\beta H}\right], \tag{96}$$

where H is the Hamiltonian of the system, Tr denotes the trace over the Hilbert space of quantum mechanical states, and

$$\beta = \frac{1}{k_B T}. \tag{97}$$

Ensemble averages of the quantum mechanical observable $\mathcal{O}$ are given by

$$\langle \mathcal{O} \rangle_\beta = \frac{1}{Z(\beta)} \mathrm{Tr}\left[e^{-\beta H}\mathcal{O}\right]. \tag{98}$$

Taking the trace over a basis of eigenstates of H with $H|n\rangle = E_n|n\rangle$ gives

$$\begin{aligned} \langle \mathcal{O} \rangle_\beta &= \frac{1}{Z(\beta)} \sum_n e^{-\beta E_n} \langle n|\mathcal{O}|n\rangle \ , \\ Z(\beta) &= \sum_n e^{-\beta E_n}. \end{aligned} \tag{99}$$

Assuming that the ground state of H is non-degenerate we have

$$\lim_{T\to 0} \langle \mathcal{O} \rangle_\beta = \langle 0|\mathcal{O}|0\rangle \ , \tag{100}$$

where $|0\rangle$ is the ground state of the system. Let us consider a QM particle with Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}), \tag{101}$$

coupled to a heat bath at temperature T. The partition function can be written in a basis of position eigenstates

$$Z(\beta) = \int dx \langle x|e^{-\beta H}|x\rangle = \int dx \int dx' \ \langle x|x'\rangle \ \langle x'|e^{-\beta H}|x\rangle. \tag{102}$$

Here

$$\langle x'|e^{-\beta H}|x\rangle \tag{103}$$

is very similar to the propagator

$$\langle x'|e^{-\frac{i(t-t_0)}{\hbar}H}|x\rangle. \tag{104}$$

Formally (103) can be viewed as the propagator in *imaginary time* $\tau = it$, where we consider propagation from $\tau = 0$ to $\tau = \beta\hbar$. Using this interpretation we can follow through precisely the same steps as before and obtain

$$\langle x_N|e^{-\beta H}|x_0\rangle = \lim_{N\to\infty} \left[\frac{m}{2\pi\hbar\epsilon}\right]^{\frac{N}{2}} \int dx_1 \dots dx_{N-1} \exp\left(-\frac{\epsilon}{\hbar}\sum_{n=0}^{N-1} \frac{m}{2}\left(\frac{x_{n+1}-x_n}{\epsilon}\right)^2 + V(x_n)\right), \tag{105}$$

where now

$$\epsilon = \frac{\hbar\beta}{N}. \tag{106}$$

We again can interpret this in terms of a sum over paths $x(\tau)$ with

$$x(\tau_n) = x_n \ , \quad \tau_n = n\epsilon. \tag{107}$$

Going over to a continuum description we arrive at an imaginary-time functional integral

$$\boxed{\langle x_N|e^{-\beta H}|x_0\rangle = \mathcal{N}\int \mathcal{D}x(\tau)\ e^{-\frac{1}{\hbar}S_E[x(\tau)]},} \tag{108}$$

where S_E is called *Euclidean action*

$$S_E[x(\tau)] = \int_0^{\hbar\beta} d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)\right], \tag{109}$$

and the path integral is over all paths that start at x_0 and end at x_N. Substituting (108) into the expression for the partition function we find that

$$\boxed{Z(\beta) = \mathcal{N}\int \mathcal{D}x(\tau)\ e^{-\frac{1}{\hbar}S_E[x(\tau)]},} \tag{110}$$

where we integrate over all *periodic paths*

$$x(\hbar\beta) = x(0). \tag{111}$$

The restriction to periodic paths arises because $Z(\beta)$ is a trace. Please note that the notation $\int \mathcal{D}x(\tau)$ means very different things in (108) and (110), as a result of involving very different classes of paths that are "integrated over". In the first case the path integral is over all paths from x_0 to x_N, in the latter over all periodic paths starting an an arbitrary position. In practice it is always clear from the context what paths are involved, and hence this ambiguous notation should not cause any confusion.

3.1 Harmonic Oscillator at $T > 0$: a first encounter with Generating Functionals

We now consider the simplest case of the potential $V(x)$, the harmonic oscillator

$$H = \frac{\hat{p}^2}{2m} + \frac{\kappa}{2}\hat{x}^2. \tag{112}$$

The physical quantities we want to work out are the averages of powers of the position operator

$$\langle \hat{x}^n\rangle_\beta = \frac{\int dx\ \langle x|e^{-\beta H}\hat{x}^n|x\rangle}{\int dx\langle x|e^{-\beta H}|x\rangle} = \frac{\int dx\ x^n\ \langle x|e^{-\beta H}|x\rangle}{\int dx\langle x|e^{-\beta H}|x\rangle}. \tag{113}$$

If we know all these moments, we can work out the probability distribution for a position measurement giving a particular result x. At zero temperature this is just given by the absolute value squared of the ground state wave function. The coupling to the heat bath will generate "excitations" of the harmonic oscillator and thus affect this probability distribution. We have

$$\langle x|e^{-\beta H}|x\rangle = \mathcal{N}\int \mathcal{D}x(\tau)\ e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + \frac{\kappa}{2}x^2\right]}, \tag{114}$$

where the path integral is over all paths with $x(0) = x(\beta\hbar)$. Integrating by parts we can write the action as

$$-\frac{1}{\hbar}S_E[x(\tau)] = -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + \frac{\kappa}{2}x^2\right] = -\frac{1}{2}\int_0^{\hbar\beta} d\tau\ x(\tau)\hat{D}x(\tau) - \frac{m}{2\hbar}x(\tau)\dot{x}(\tau)\Big|_0^{\hbar\beta}, \tag{115}$$

where

$$\hat{D} = -\frac{m}{\hbar}\frac{d^2}{d\tau^2} + \frac{\kappa}{\hbar}. \tag{116}$$

The contributions from the integration boundaries in (115) don't play a role in the logic underlying the following steps leading up to (124) and work out in precisely the same way as the "bulk" contributions. In order to show that we're not dropping anything important we'll keep track of them anyway. We now define the *generating functional*

$$W[J] \equiv \mathcal{N} \int \mathcal{D}x(\tau)\; e^{-\frac{1}{\hbar}S_E[x(\tau)]+\int_0^{\hbar\beta} d\tau\; J(\tau)x(\tau)}. \tag{117}$$

Here the functions $J(\tau)$ are called *sources*. The point of the definition (117) is that we can obtain $\langle \hat{x}^n \rangle_\beta$ by taking functional derivatives

$$\langle \hat{x}^n \rangle_\beta = \frac{1}{W[0]} \frac{\delta}{\delta J(0)} \cdots \frac{\delta}{\delta J(0)} \bigg|_{J=0} W[J]. \tag{118}$$

We now could go ahead and calculate the generating functional by going back to the definition of the the path integral in terms of a multidimensional Gaussian integral. In practice we manipulate the path integral itself as follows. Apart from the contribution from the integration boundaries the structure of (115) is completely analogous to the one we encountered for Gaussian integrals, cf (31). The change of variables (32) suggests that we should shift our "integration variables" by a term involving the inverse of the integral operator $\hat{D}$. The latter corresponds to the Green's function defined by

$$\hat{D}_\tau G(\tau - \tau') = \delta(\tau - \tau') \;, \quad G(0) = G(\beta\hbar). \tag{119}$$

We then change variables in the path integral in order to "complete the square"

$$y(\tau) = x(\tau) - \int d\tau'\; G(\tau - \tau')J(\tau'). \tag{120}$$

Under this change of variables we have

$$\begin{aligned} \int d\tau\; x(\tau)\hat{D}_\tau x(\tau) - 2\int d\tau\; x(\tau)J(\tau) \;\; &= \;\; \int d\tau\; y(\tau)\hat{D}_\tau y(\tau) - \int d\tau d\tau'\; J(\tau)G(\tau-\tau')J(\tau') \\ &\quad + \text{boundary terms.} \end{aligned} \tag{121}$$

Exercise

Verify that

$$\begin{aligned} \int d\tau\; y(\tau)\hat{D}_\tau y(\tau) \;\; &= \;\; \int d\tau\; x(\tau)\hat{D}_\tau x(\tau) + \int d\tau d\tau' d\tau''\; G(\tau-\tau')J(\tau')\hat{D}_\tau G(\tau-\tau'')J(\tau'') \\ &\quad - \int d\tau d\tau' \Big[x(\tau)\hat{D}_\tau G(\tau-\tau')J(\tau') + G(\tau-\tau')J(\tau')\hat{D}_\tau x(\tau) \Big] \\ &= \int d\tau\; x(\tau)\hat{D}_\tau x(\tau) + \int d\tau d\tau'\; G(\tau-\tau')J(\tau')J(\tau) - 2\int d\tau\; x(\tau)J(\tau) \\ &\quad + \frac{m}{\hbar} x(\tau)\dot{x}(\tau)\Big|_0^{\hbar\beta} - \frac{m}{\hbar} y(\tau)\dot{y}(\tau)\Big|_0^{\hbar\beta}, \end{aligned} \tag{122}$$

In the last step you need to use (119) and integrate by parts twice to simplify the last term in the second line.

Exercise

Putting everything together we arrive at

$$-\frac{1}{\hbar}S_E[x(\tau)] + \int_0^{\hbar\beta} d\tau\; J(\tau)x(\tau) = -\frac{1}{\hbar}S_E[y(\tau)] + \frac{1}{2}\int_0^{\hbar\beta} d\tau d\tau' J(\tau)G(\tau-\tau')J(\tau'). \tag{123}$$

On the other hand, the Jacobian of the change of variables (120) is 1 as we are shifting all paths by the same constant (you can show this directly by going back to the definition of the path integral in terms of multiple Gaussian integrals). Hence we have $\mathcal{D}y(\tau) = \mathcal{D}x(\tau)$ and our generating functional becomes

$$\boxed{W[J] = W[0]\; e^{\frac{1}{2}\int d\tau d\tau'\; J(\tau)G(\tau-\tau')J(\tau')}.} \tag{124}$$

Now we are ready to calculate (118). The average position is zero

$$\langle \hat{x} \rangle_\beta = \frac{1}{W[0]} \frac{\delta}{\delta J(0)} \bigg|_{J=0} W[J] = \frac{1}{2W[0]} \int d\tau d\tau' \left[\delta(\tau) G(\tau - \tau') J(\tau') + J(\tau) G(\tau - \tau') \delta(\tau') \right] W[J] \bigg|_{J=0} = 0. \tag{125}$$

Here we have used that

$$\frac{\delta J(\tau)}{\delta J(\tau')} = \delta(\tau - \tau'). \tag{126}$$

The expression (125) vanishes, because we have a "left over" J and obtain zero when setting all sources to zero in the end of the calculation. By the same mechanism we have

$$\langle \hat{x}^{2n+1} \rangle_\beta = 0. \tag{127}$$

Next we turn to

$$\begin{aligned} \langle \hat{x}^2 \rangle_\beta &= \frac{1}{W[0]} \frac{\delta}{\delta J(0)} \frac{\delta}{\delta J(0)} \bigg|_{J=0} W[J] \\ &= \frac{1}{W[0]} \frac{\delta}{\delta J(0)} \bigg|_{J=0} \frac{1}{2} \int d\tau d\tau' \left[\delta(\tau) G(\tau - \tau') J(\tau') + J(\tau) G(\tau - \tau') \delta(\tau') \right] W[J] = G(0). \end{aligned} \tag{128}$$

So the mean square deviation of the oscillator's position is equal to the Green's function evaluated at zero.

3.1.1 Imaginary Time Green's Function of the Harmonic Oscillator

To determine $G(\tau)$ we need to solve the differential equation (119). As $G(0) = G(\beta\hbar)$ we are dealing with a periodic function and therefore may employ a Fourier expansion

$$G(\tau) = \frac{1}{\sqrt{\beta\hbar}} \sum_{n=-\infty}^{\infty} g_n e^{i\omega_n \tau}, \tag{129}$$

where the *Matsubara frequencies* ω_n are

$$\omega_n = \frac{2\pi n}{\beta\hbar}. \tag{130}$$

Substituting this into the differential equation gives

$$\hat{D} G(\tau) = \frac{1}{\sqrt{\beta\hbar}} \sum_{n=-\infty}^{\infty} g_n e^{i\omega_n \tau} \left[\frac{m\omega_n^2}{\hbar} + \frac{\kappa}{\hbar} \right] = \delta(\tau). \tag{131}$$

Taking the integral $\int_0^{\hbar\beta} d\tau e^{-i\omega_k \tau}$ on both sides fixes the Fourier coefficients and we obtain

$$G(\tau) = \frac{1}{\beta\kappa} \sum_{n=-\infty}^{\infty} \frac{\omega^2}{\omega^2 + \omega_n^2} e^{i\omega_n \tau} \ , \tag{132}$$

where $\omega = \sqrt{\kappa/m}$. Using contour integration techniques this can be rewritten as

$$G(\tau) = \frac{\hbar\omega}{2\kappa} \left[\frac{e^{\omega|\tau|}}{e^{\hbar\beta\omega} - 1} + \frac{e^{-\omega|\tau|}}{1 - e^{-\hbar\beta\omega}} \right]. \tag{133}$$

Setting $\tau = 0$ gives

$$G(0) = \frac{\hbar\omega}{2\kappa \tanh\left(\beta\hbar\omega/2\right)} = \frac{\hbar\omega}{\kappa} \left[\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2} \right]. \tag{134}$$

We can relate this result to things we already know: using equipartition

$$\langle H\rangle_\beta = \langle T\rangle_\beta + \langle V\rangle_\beta = 2\langle V\rangle_\beta = \kappa\langle \hat{x}^2\rangle_\beta = \kappa G(0), \tag{135}$$

we find that the average energy of the oscillator at temperature T is

$$\langle H\rangle_\beta = \hbar\omega\left[\frac{1}{e^{\beta\hbar\omega}-1}+\frac{1}{2}\right]. \tag{136}$$

Recalling that the Hamiltonian of the harmonic oscillator can be expressed as

$$H = \hbar\omega(\hat{n}+\frac{1}{2}), \tag{137}$$

where $\hat{n} = a^\dagger a$ is the number operator, we recover the Bose-Einstein distribution

$$\langle \hat{n}\rangle_\beta = \frac{1}{e^{\beta\hbar\omega}-1}. \tag{138}$$

3.2 Homework Question 6

Question 6. In this question the objective is to evaluate the Feynman path integral in one of the relatively few cases, besides those treated in lectures, for which exact results can be obtained. The system we consider consists of a particle of mass m moving on a circle of circumference L. The quantum Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

and wavefunctions obey $\psi(x+L)=\psi(x)$. We want to determine the imaginary time propagator

$$\langle x_1|\exp(-\beta H)|x_2\rangle\,.$$

a) What are the eigenstates and eigenvalues of H? As we are dealing with a free particle, we can determine the propagator as in the lectures in a simple way by inserting resolutions of the identity in terms of the eigenstates of H. Show that this leads to the following result

$$\langle x_1|\exp(-\beta H)|x_2\rangle = \sum_{n=-\infty}^{\infty}\frac{1}{L}\exp\left(-\frac{\beta(2\pi n)^2\hbar^2}{2mL^2}+2\pi i n\frac{[x_1-x_2]}{L}\right). \tag{139}$$

b) Next, approach this using a path integral in which paths $x(\tau)$ for $0\le\tau\le\beta\hbar$ satisfy the boundary conditions $x(0)=x_1$ and $x(\beta\hbar)=x_2$. The special feature of a particle moving on a circle is that such paths may wind any integer number l times around the circle. To build in this feature, write

$$x(\tau) = x_1 + \frac{\tau}{\beta\hbar}[(x_2-x_1)+lL] + s(\tau),$$

where the contribution $s(\tau)$ obeys the simpler boundary conditions $s(0)=s(\beta\hbar)=0$ and does *not* wrap around the circle. Show that the Euclidean action for the system on such a path is

$$S[x(\tau)] = S_l + S[s(\tau)] \qquad \text{where} \qquad S_l = \frac{m}{2\beta\hbar}[(x_2-x_1)+lL]^2 \qquad \text{and} \qquad S[s(\tau)] = \int_0^{\beta\hbar}\mathrm{d}\tau\frac{m}{2}\left(\frac{\mathrm{d}s}{\mathrm{d}\tau}\right)^2.$$

c) using the results of b) show that

$$\langle x_1|\exp(-\beta H)|x_2\rangle \;= \mathcal{Z}_0\sum_{l=-\infty}^{\infty}\exp\left(-\frac{m}{2\beta\hbar^2}[(x_1-x_2)+lL]^2\right), \tag{140}$$

where $\mathcal{Z}_0$ is the diagonal matrix element $\langle x|\mathrm{e}^{-\beta H}|x\rangle$ for a *free* particle (i.e. without periodic boundary conditions) moving in one dimension.
d) Argue on the basis of the result you obtained in Qu 3. for the propagator of a free particle that

$$\mathcal{Z}_0 = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2} . \tag{141}$$

e) Show that the expressions in Eq. (139) and Eq. (140) are indeed equal. To do so, you should use the *Poisson summation formula*

$$\sum_{l=-\infty}^{\infty} \delta(y-l) = \sum_{n=-\infty}^{\infty} \mathrm{e}^{-2\pi i n y}$$

(think about how to justify this). Introduce the left hand side of this expression into Eq. (140) by using the relation, valid for any smooth function $f(y)$,

$$\sum_{l=-\infty}^{\infty} f(l) = \int_{-\infty}^{\infty} \mathrm{d}y \sum_{l=-\infty}^{\infty} \delta(y-l) f(y)\,,$$

substitute the right hand side of the summation formula, carry out the (Gaussian) integral on y, and hence establish the required equality.

3.3 Correlation Functions

It is clear from the above that we can calculate more general quantities from the generating functional $W[J]$, namely

$$\frac{1}{W[0]} \prod_{j=1}^{n} \frac{\delta}{\delta J(\tau_j)}\bigg|_{J=0} W[J] = \frac{\mathcal{N}}{W[0]} \int \mathcal{D}x(\tau) \prod_{j=1}^{n} x(\tau_j)\; e^{-\frac{1}{\hbar} S_E[x(\tau)]} \tag{142}$$

What is their significance? Graphically, the path integral in (142) is represented in Fig. 2. It consists of

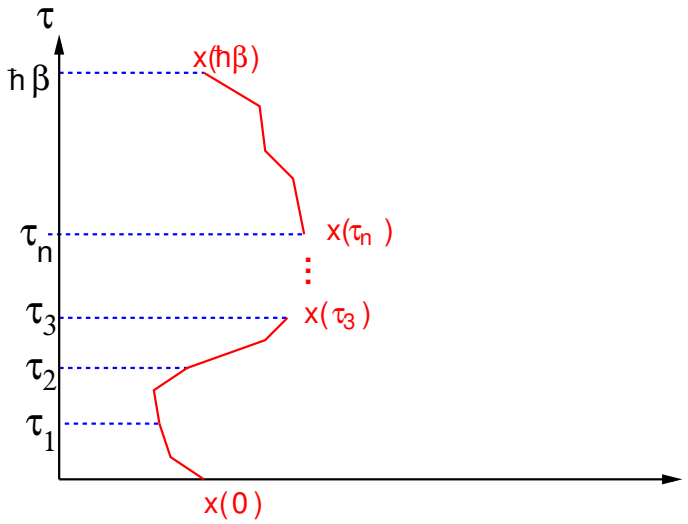


Figure 2: Path integral corresponding to (142).

several parts. The first part corresponds to propagation from $x(0)$ to $x(\tau_1)$ and the associated propagator is

$$\langle x(\tau_1)|e^{-H\tau_1/\hbar}|x(0)\rangle. \tag{143}$$

The second part corresponds to propagation from $x(\tau_1)$ to $x(\tau_2)$, and we have a multiplicative factor of $x(\tau_1)$ as well. This is equivalent to a factor

$$\langle x(\tau_2)|e^{-H(\tau_2-\tau_1)/\hbar}\hat{x}|x(\tau_1)\rangle. \tag{144}$$

Repeating this analysis for the other pieces of the path we obtain

$$\left[\prod_{j=1}^{n}\langle x(\tau_{j+1})|e^{-H(\tau_{j+1}-\tau_j)/\hbar}\hat{x}|x(\tau_j)\rangle\right]\langle x(\tau_1)|e^{-H\tau_1/\hbar}|x(0)\rangle\ , \tag{145}$$

where $\tau_{n+1} = \hbar\beta$. Finally, in order to represent the full path integral (142) we need to integrate over the intermediate positions $x(\tau_j)$ and impose periodicity of the path. Using that $\mathbf{1} = \int dx|x\rangle\langle x|$ and that $W[0] = Z(\beta)$ we arrive at

$$\begin{aligned}\frac{1}{Z(\beta)}\int dx(0)\langle x(0)|e^{-H(\beta-\tau_n)/\hbar}\hat{x}e^{-H(\tau_n-\tau_{n-1})/\hbar}\hat{x}\ldots\hat{x}e^{-H(\tau_2-\tau_1)/\hbar}\hat{x}e^{-H\tau_1/\hbar}|x(0)\rangle \\ = \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}\bar{x}(\tau_n)\bar{x}(\tau_{n-1})\ldots\bar{x}(\tau_1)\right],\end{aligned} \tag{146}$$

where we have defined operators

$$\bar{x}(\tau_j) = e^{H\tau_j/\hbar}\hat{x}e^{-H\tau_j/\hbar}. \tag{147}$$

There is one slight subtlety: in the above we have used implicitly that $\tau_1 < \tau_2 < \ldots < \tau_n$. On the other hand, our starting point (142) is by construction symmetric in the τ_j. The way to fix this is to introduce a *time-ordering* operation T_τ, which automatically arranges operators in the "right" order. For example

$$T_\tau\bar{x}(\tau_1)\bar{x}(\tau_2) = \theta(\tau_1-\tau_2)\bar{x}(\tau_1)\bar{x}(\tau_2) + \theta(\tau_2-\tau_1)\bar{x}(\tau_2)\bar{x}(\tau_1), \tag{148}$$

where $\theta(x)$ is the Heaviside theta function. Then we have

$$\boxed{\frac{1}{W[0]}\prod_{j=1}^{n}\frac{\delta}{\delta J(\tau_j)}\bigg|_{J=0}W[J] = \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}T_\tau\bar{x}(\tau_1)\bar{x}(\tau_2)\ldots\bar{x}(\tau_n)\right].} \tag{149}$$

Finally, if we *analytically continue* from imaginary time to real time $\tau_j \to it_j$, the operators $\bar{x}(\tau)$ turn into *Heisenberg-picture* operators

$$\hat{x}(t) \equiv e^{\frac{it}{\hbar}H}\hat{x}e^{-\frac{it}{\hbar}H}. \tag{150}$$

The quantities that we get from (149) after analytic continuation are called *n-point correlation functions*

$$\boxed{\langle T\hat{x}(t_1)\hat{x}(t_2)\ldots\hat{x}(t_n)\rangle_\beta \equiv \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}T\hat{x}(t_1)\hat{x}(t_2)\ldots\hat{x}(t_n)\right].} \tag{151}$$

Here T is a time-ordering operator that arranges the $\hat{x}(t_j)$'s in chronologically increasing order from right to left. Such correlation functions are the central objects in both quantum field theory and many-particle quantum physics.

3.3.1 Wick's Theorem

Recalling that

$$W[J] = W[0]\ e^{\frac{1}{2}\int d\tau d\tau'\ J(\tau)G(\tau-\tau')J(\tau')}, \tag{152}$$

then taking the functional derivatives, and finally setting all sources to zero we find that

$$\frac{1}{W[0]}\prod_{j=1}^{n}\frac{\delta}{\delta J(\tau_j)}\bigg|_{J=0} W[J] = \sum_{P(1,\ldots,n)} G(\tau_{P_1}-\tau_{P_2})\ldots G(\tau_{P_{n-1}}-\tau_{P_n})\ . \tag{153}$$

Here the sum is over all possible pairings of $\{1,2,\ldots,n\}$ and $G(\tau)$ is the Green's function (132). In particular we have

$$\langle T_\tau \bar{x}(\tau_1)\bar{x}(\tau_2)\rangle_\beta = G(\tau_1-\tau_2). \tag{154}$$

The fact that for "Gaussian theories" [3] like the harmonic oscillator n-point correlation functions can be expressed as simple products over 2-point functions is known as *Wick's theorem.*

3.4 Probability distribution of position

Using Wick's theorem it is now straightforward to calculate all moments $\langle \hat{x}^{2n}\rangle_\beta$ for the harmonic oscillator. It is instructive to calculate the corresponding probability distribution directly. Let us first work out the relevant expectation value to consider. Let $|\psi\rangle$ be an arbitrary state and consider

$$\langle\psi|\delta(\hat{x}-x_0)|\psi\rangle = \int dx \langle\psi|\delta(\hat{x}-x_0)|x\rangle\langle x|\psi\rangle = \int dx\ \delta(x-x_0)\langle\psi|x\rangle\langle x|\psi\rangle = |\psi(x_0)|^2. \tag{155}$$

So the expectation value of the delta-function indeed gives the correct result for the probability distribution of a position measurement, namely the absolute value squared of the wave function. We then have

$$\begin{aligned}\langle\delta(\hat{x}-x_0)\rangle_\beta &= \int_{-\infty}^{\infty}\frac{dk}{2\pi}\langle e^{ik(\hat{x}-x_0)}\rangle_\beta \\ &= \int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{-ikx_0}\frac{\mathcal{N}}{W[0]}\int\mathcal{D}x(\tau)\ e^{-\frac{1}{2}\int_0^{\hbar\beta}d\tau\ x(\tau)\hat{D}x(\tau)+\int_0^{\hbar\beta}d\tau\ x(\tau)ik\delta(\tau)}.\end{aligned} \tag{156}$$

This is a special case of our generating functional, where the source is given by $J(\tau)=ik\delta(\tau)$. We therefore can use (124) to obtain

$$\begin{aligned}\langle\delta(\hat{x}-x_0)\rangle_\beta &= \int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{-ikx_0}\frac{W[ik\delta(\tau)]}{W[0]} = \int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{-ikx_0}e^{\frac{1}{2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\left(ik\delta(\tau)\right)G(\tau-\tau')\left(ik\delta(\tau')\right)} \\ &= \frac{1}{\sqrt{2\pi G(0)}}e^{-x_0^2/2G(0)}.\end{aligned} \tag{157}$$

To go from the first to the second line we have taken the integrals over τ and τ' (which are straightforward because of the two delta functions) and finally carried out the k-integral using the one dimensional version of (34). We see that our probability distribution is a simple Gaussian with a variance that depends on temperature through $G(0)$. Note that at zero temperature (157) reduces, as it must, to $|\psi_0(x_0)|^2$, where $\psi_0(x)$ is the ground state wave function of the harmonic oscillator.

3.5 Perturbation Theory and Feynman Diagrams

Let us now consider the anharmonic oscillator

$$H = \frac{\hat{p}^2}{2m}+\frac{\kappa}{2}\hat{x}^2+\frac{\lambda}{4!}\hat{x}^4. \tag{158}$$

As you know from QM2, this Hamiltonian is no longer exactly solvable. What we want to do instead is perturbation theory for small $\lambda>0$. As the Hamiltonian is of the form $H=\frac{\hat{p}^2}{2m}+V(\hat{x})$ our previous construction of the path integral applies. Our generating functional becomes

$$W_\lambda[J] = \mathcal{N}\int\mathcal{D}x(\tau)\ e^{-\frac{1}{\hbar}S_E[x(\tau)]+\int_0^{\hbar\beta}d\tau\ J(\tau)x(\tau)-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta}d\tau\ x^4(\tau)}. \tag{159}$$

[3] These are theories in which the Lagrangian is quadratic in the generalized co-ordinates.

The partition function is

$$Z_\lambda(\beta) = W_\lambda[0] \; . \tag{160}$$

The idea is to expand (159) perturbatively in powers of λ

$$\begin{aligned} W_\lambda[J] &= \mathcal{N}\int \mathcal{D}x(\tau)\; \left[1 - \frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau'\; x^4(\tau') + \ldots\right] e^{-\frac{1}{\hbar}S_E[x(\tau)] + \int_0^{\hbar\beta} d\tau\; J(\tau)x(\tau)} \\ &= \mathcal{N}\int \mathcal{D}x(\tau)\; \left[1 - \frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau'\; \left[\frac{\delta}{\delta J(\tau')}\right]^4 + \ldots\right] e^{-\frac{1}{\hbar}S_E[x(\tau)] + \int_0^{\hbar\beta} d\tau\; J(\tau)x(\tau)} \\ &= \mathcal{N}\int \mathcal{D}x(\tau)\; e^{-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau'\; \left[\frac{\delta}{\delta J(\tau')}\right]^4} e^{-\frac{1}{\hbar}S_E[x(\tau)] + \int_0^{\hbar\beta} d\tau\; J(\tau)x(\tau)} \\ &= e^{-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau'\; \left[\frac{\delta}{\delta J(\tau')}\right]^4} W_0[J]. \end{aligned} \tag{161}$$

We already know $W_0[J]$

$$W_0[J] = W_0[0]\; e^{\frac{1}{2}\int d\tau d\tau'\; J(\tau)G(\tau-\tau')J(\tau')}, \tag{162}$$

which will enable us to work out a perturbative expansion very efficiently.

3.5.1 Partition Function of the anharmonic oscillator

By virtue of (160) the perturbation expansion for $Z_\lambda(\beta)$ is

$$\begin{aligned} Z_\lambda(\beta) &= e^{-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau'\; \left[\frac{\delta}{\delta J(\tau')}\right]^4} W_0[J]\Big|_{J=0} = Z_0(\beta) - \frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau'\; \left[\frac{\delta}{\delta J(\tau')}\right]^4\Big|_{J=0} W_0[J] \\ &\qquad + \frac{1}{2}\left[\frac{\lambda}{4!\hbar}\right]^2 \int_0^{\hbar\beta} d\tau' d\tau''\; \left[\frac{\delta}{\delta J(\tau')}\right]^4 \left[\frac{\delta}{\delta J(\tau'')}\right]^4\Big|_{J=0} W_0[J] + \ldots \\ &= Z_0(\beta)\left[1 + \lambda\gamma_1(\beta) + \lambda^2\gamma_2(\beta) + \ldots\right]. \end{aligned} \tag{163}$$

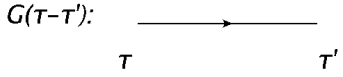
1. *First order perturbation theory.*

   Carrying out the functional derivatives gives

   $$\lambda\gamma_1(\beta) = -\frac{\lambda}{8\hbar}\int_0^{\hbar\beta} d\tau'\; [G(\tau-\tau)]^2 = -\frac{\lambda\beta}{8}\,[G(0)]^2\,. \tag{164}$$

   This contribution can be represented graphically by a *Feynman diagram.* In order to do so we introduce the following elements:

   (a) The two-point function $G(\tau-\tau')$ is represented by a line running from τ to τ'.

   (b) The *interaction vertex* $-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau$ is represented by

   Combining these two elements, we can express the integral $\lambda\gamma_1(\beta)$ by the diagram

   Here the factor of 3 is a *combinatorial factor* associated with the diagram.

2. *Second order perturbation theory.*

   To second order we obtain a number of different contributions upon taking the functional derivatives. The full second order contribution is

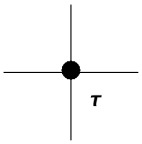


Figure 3: Graphical representation of the interaction vertex.

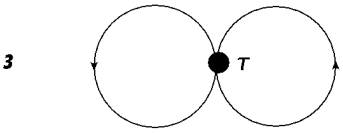


Figure 4: Feynman diagram for the 1st order perturbative contribution to the partition function.

$$\begin{aligned}\lambda^2\gamma_2(\beta) &= \frac{1}{2}\left(\frac{\lambda}{4!\hbar}\right)^2 72\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\; G(\tau-\tau)G^2(\tau-\tau')G(\tau'-\tau') \\ &+ \frac{1}{2}\left(\frac{\lambda}{4!\hbar}\right)^2 24\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\; G^4(\tau-\tau') \\ &+ \frac{1}{2}\left(\frac{\lambda}{4!\hbar}\right)^2 9\left[\int_0^{\hbar\beta}d\tau G^2(\tau-\tau)\right]^2 . \end{aligned} \tag{165}$$

The corresponding Feynman diagrams are shown in Fig.5. They come in two types: the first two are *connected*, while the third is *disconnected*.

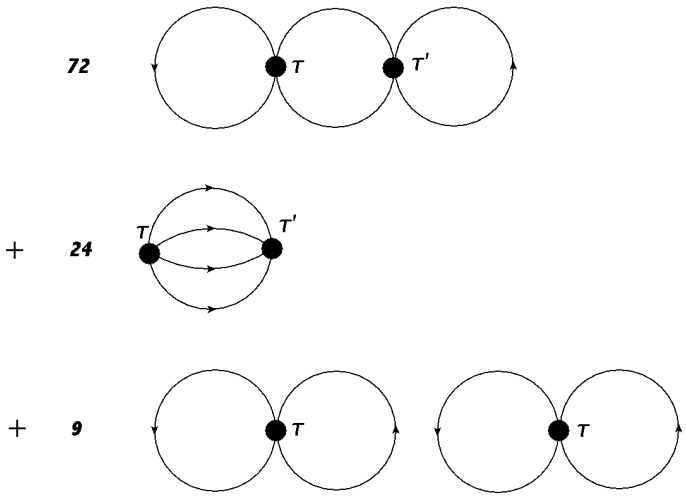


Figure 5: Feynman diagram for the 2nd order perturbative contribution to the partition function.

The point about the Feynman diagrams is that rather than carrying out functional derivatives and then representing various contributions in diagrammatic form, in practice we do the calculation by writing down the diagrams *first* and then working out the corresponding integrals! How do we know what diagrams to draw? As we are dealing with the partition function, we can never produce a diagram with a line sticking out: all (imaginary) times must be integrated over. Such diagrams are sometimes called *vacuum diagrams*. Now, at first order in λ, we only have a single vertex, i.e. a single integral over τ. The combinatorics works out as follows:

1. We have to count the number of ways of connecting a single vertex to two lines, that reproduce the diagram we want.

2. Let us introduce a short-hand notation

$$W[J] = W[0]e^{\frac{1}{2}J_1 G_{12} J_2} = W[0]\left[1 + \frac{1}{2}J_1 G_{12} J_2 + \frac{1}{2^3}J_1 G_{12} J_2 J_3 G_{34} J_4 + \dots\right]. \tag{166}$$

   The last term we have written is the one that gives rise to our diagram, so we have a factor

$$\frac{1}{2^3} \tag{167}$$

   to begin with.

3. Now, the combinatorics of acting with the functional derivatives is the same as the one of connecting a single vertex to two lines. There are 4 ways of connecting the first line to the vertex, and 3 ways of connecting the second. Finally there are two ways of connecting the end of the first line to the vertex as well. The end of the second line must then also be connected to the vertex to give our diagram, but there is no freedom left. Altogether we obtain a factor of 24. Combining this with the factor of 1/8 we started with gives a *combinatorial factor* of 3. That's a Bingo!

3.6 Homework Question 7

Question 7. Anharmonic Oscillator. Consider the anharmonic oscillator

$$H(\lambda_1, \lambda_2) = \frac{\hat{p}^2}{2m} + \frac{\kappa}{2}\hat{x}^2 + \frac{\lambda_1}{3!}\hat{x}^3 + \frac{\lambda_2}{4!}\hat{x}^4. \tag{168}$$

where $\kappa, \lambda_{1,2} > 0$ and $\lambda_1^2 - 3\kappa\lambda_2 < 0$. Define a generating functional by

$$W_{\lambda_1,\lambda_2}[J] = \mathcal{N}\int \mathcal{D}x(\tau)\; e^{\left\{\int_0^{\hbar\beta} d\tau\left[-\frac{1}{\hbar}S_E[x(\tau)] + J(\tau)x(\tau)\right] + U\left(x(\tau)\right)\right\}}, \tag{169}$$

where

$$U\big(x(\tau)\big) = -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\left[\frac{\lambda_1}{3!}x^3(\tau) + \frac{\lambda_2}{4!}x^4(\tau)\right], \quad \hat{D} = -\frac{m}{\hbar}\frac{d^2}{d\tau^2} + \frac{\kappa}{\hbar}. \tag{170}$$

a) Show that the partition function is equal to

$$Z_{\lambda_1,\lambda_2}(\beta) = W_{\lambda_1,\lambda_2}[0]. \tag{171}$$

b) Show that the generating functional can be expressed in the form

$$W_{\lambda_1,\lambda_2}[J] = \exp\left(U\Big(\frac{\delta}{\delta J(\tau)}\Big)\right) W_{0,0}[J]. \tag{172}$$

c) Determine the first order perturbative corrections in λ_1 and λ_2 to the partition function. Draw the corresponding Feynman diagrams.
d) Determine the perturbative correction to the partition function proportional to λ_1^2. Draw the corresponding Feynman diagrams. Are there corrections of order $\lambda_1\lambda_2$?
e)* Determine the first order corrections to the two-point function

$$\langle T_\tau \bar{x}(\tau_1)\bar{x}(\tau_2)\rangle_\beta. \tag{173}$$

Draw the corresponding Feynman diagrams. What diagrams to you get in second order in perturbation theory?

Part II
Path Integrals and Transfer Matrices

4 Relation of D dimensional quantum systems to $D+1$ dimensional classical ones

Let's start by defining what we mean by the spatial "dimension" D of a system. Let us do this by considering a (quantum) field theory. There the basic objects are fields, that depend on time and are defined at all points of a D-dimensional space. This value of D defines what we mean by the spatial dimension. For example, in electromagnetism we have $D = 3$. In this terminology a single quantum mechanical particle or spin are zero-dimensional systems. On the other hand, a linear chain of spins is a one-dimensional system, while a bcc lattice of spins has $D = 3$. Interestingly, there is a representation of D dimensional quantum systems in terms of $D+1$ dimensional classical ones. We will now establish this for the particular case of the simple quantum mechanical harmonic oscillator.

4.1 Some Facts from Statistical Physics

Consider a classical many-particle system coupled to a heat bath at temperature T. The *partition function* is defined as

$$Z = \sum_{\text{configurations C}} e^{-\beta E(C)} , \qquad \beta = \frac{1}{k_B T}. \tag{174}$$

Here the sum is over all possible configurations C, and $E(C)$ is the corresponding energy. Thermal averages of observables are given by

$$\langle \mathcal{O} \rangle_\beta = \frac{1}{Z} \sum_{\text{configurations C}} \mathcal{O}(C) e^{-\beta E(C)} , \tag{175}$$

where $\mathcal{O}(C)$ is the value of the observable $\mathcal{O}$ in configuration C. The average energy is

$$E = \frac{1}{Z} \sum_{\text{configurations C}} E(C) e^{-\beta E(C)} = -\frac{\partial}{\partial \beta} \ln(Z). \tag{176}$$

The *free energy* is

$$F = -k_B T \ln(Z). \tag{177}$$

The *entropy* is

$$S = \frac{E - F}{T} = k_B \ln(Z) - k_B \beta \frac{\partial}{\partial \beta} \ln(Z) = k_B \frac{\partial}{\partial T} \left[T \ln(Z) \right]. \tag{178}$$

4.2 Quantum Mechanical Particle

Let us revisit the path-integral representation (108) for the partition function of our QM particle at temperature β

$$Z(\beta) = \lim_{N \to \infty} \int dx \left[\frac{m}{2\pi\hbar\epsilon} \right]^{\frac{N}{2}} \int dx_1 \dots dx_{N-1} \exp\left(-\frac{\epsilon}{\hbar} \sum_{n=0}^{N-1} \frac{m}{2} \left(\frac{x_{n+1} - x_n}{\epsilon} \right)^2 + V(x_n) \right), \tag{179}$$

where we have set $x_0 = x_N = x$. For a given value of N, this can be interpreted as the partition function of N classical degrees of freedom x_j, that can be thought of as deviations of classical particles from their equilibrium positions, cf. Fig. 6. In this interpretation $V(x_j)$ is simply a potential energy associated with moving the j^{th} particle a distance x_j away from its equilibrium position, while $\frac{m}{2}(x_{n+1} - x_n)^2/\epsilon^2$ describes

Figure 6: Periodic array of classical particles.

an interaction energy that favours equal displacements, i.e. $x_n = x_{n+1}$. Importantly, the temperature T_{cl} of this one-dimensional classical model equals

$$k_B T_{cl} = \frac{\hbar}{\epsilon} = N k_B T. \tag{180}$$

So for large values of N (and fixed T) this temperature is very large. A convenient way for working out partition functions in classical statistical mechanics is by using *transfer matrices*. In the case at hand, this is defined as an integral operator $\hat{T}$ with kernel

$$\begin{aligned} T(x,x') &= \sqrt{\frac{m}{2\pi\epsilon\hbar}} e^{-\frac{\beta}{N} E_{\rm cl}(x,x')} \ , \\ E_{\rm cl}(x,x') &= \frac{m}{2}\left(\frac{x-x'}{\epsilon}\right)^2 + \frac{V(x)+V(x')}{2}. \end{aligned} \tag{181}$$

The integral operator $\hat{T}$ acts on functions $f(x)$ as

$$(\hat{T} * f)(x) = \int dx' \ T(x,x') f(x'). \tag{182}$$

In terms of this transfer matrix the partition function can be written as

$$\begin{aligned} Z(\beta) &= \lim_{N\to\infty} \int dx dx_1 \dots dx_{N-1} \ T(x,x_1) T(x_1,x_2) \dots T(x_{N-1},x) \\ &= \lim_{N\to\infty} \int dx \ T^N(x,x) = \lim_{N\to\infty} {\rm Tr}(\hat{T}^N). \end{aligned} \tag{183}$$

By construction $\hat{T}$ is a real, symmetric operator and can therefore be diagonalized. Hence the partition function can be expressed in terms of the eigenvalues of $\hat{T}$ using

$${\rm Tr}(\hat{T}^N) = \sum_n \lambda_n^N. \tag{184}$$

In order to get a clearer idea how to use transfer matrices in statistical mechanics problems we now turn to a simpler example, the celebrated *Ising model*. This is in fact *the* key paradigm in the theory of phase transitions.

5 The Ising Model

Ferromagnetism is an interesting phenomenon in solids. Some metals (like Fe or Ni) are observed to acquire a finite magnetization below a certain temperature. Ferromagnetism is a fundamentally quantum mechanical effect, and arises when electron spins spontaneously align along a certain direction. The Ising model is a very crude attempt to model this phenomenon. It is defined as follows. We have a lattice in D dimensions with N sites. On each site j of this lattice sits a "spin" variable σ_j, which can take the two values ± 1. These are referred to as "spin-up" and "spin-down" respectively. A given set $\{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ specifies a *configuration*. The corresponding energy is taken to be of the form

$$E(\{\sigma_j\}) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - h \sum_{j=1}^{N} \sigma_j \ , \tag{185}$$

where $\langle ij \rangle$ denote nearest-neighbour bonds on our lattice and $J > 0$. The first term favours alignment on neighbouring spins, while h is like an applied magnetic field. Clearly, when $h = 0$ the lowest energy states are obtained by choosing all spins to be either up or down. The question of interest is whether the Ising model displays a finite temperature phase transition between a ferromagnetically ordered phase at low temperatures, and a paramagnetic phase at high temperatures.

5.1 Statistical mechanics of the Ising model

The partition function of the model is

$$Z = \sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} e^{-\beta E(\{\sigma_j\})}. \tag{186}$$

The *magnetization per site* is given by

$$m(h) = \frac{1}{N} \langle \sum_{j=1}^{N} \sigma_j \rangle_\beta = \frac{1}{N\beta} \frac{\partial}{\partial h} \ln(Z). \tag{187}$$

The *magnetic susceptibility* is defined as

$$\chi(h) = \frac{\partial m(h)}{\partial h} = \frac{1}{N\beta} \frac{\partial^2}{\partial h^2} \ln(Z). \tag{188}$$

Substituting the expression (186) for the partition function and then carrying out the derivatives it can be expressed in the form

$$\chi(h) = \frac{\beta}{N} \sum_{l,m=1}^{N} \langle \sigma_l \sigma_m \rangle_\beta - \langle \sigma_l \rangle_\beta \langle \sigma_m \rangle_\beta. \tag{189}$$

5.2 The One-Dimensional Ising Model

The simplest case is when our lattice is one-dimensional, and we impose periodic boundary conditions. The energy then reads

$$E = \sum_{j=1}^{N} \left[-J \sigma_j \sigma_{j+1} - \frac{h}{2} (\sigma_j + \sigma_{j+1}) \right] \equiv \sum_{j=1}^{N} E(\sigma_j, \sigma_{j+1}), \tag{190}$$

where we have defined

$$\sigma_{N+1} = \sigma_1. \tag{191}$$

The partition function can be expressed in the form

$$Z = \sum_{\sigma_1, \ldots, \sigma_N} \prod_{j=1}^{N} e^{-\beta E(\sigma_j, \sigma_{j+1})}. \tag{192}$$

It can be evaluated exactly by means of the *transfer matrix method*.

5.2.1 Transfer matrix approach

The general idea is to rewrite Z as a product of matrices. The transfer matrix T is taken to be a 2×2 matrix with elements

$$T_{\sigma\sigma'} = e^{-\beta E(\sigma,\sigma')}. \tag{193}$$

Its explicit form is

$$T = \begin{pmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{pmatrix} = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix}. \tag{194}$$

The partition function can be expressed in terms of the transfer matrix as follows

$$Z = \sum_{\sigma_1,\ldots,\sigma_N} T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} \ldots T_{\sigma_{N-1}\sigma_N} T_{\sigma_N\sigma_1} \tag{195}$$

As desired, this has the structure of a matrix multiplication

$$\boxed{Z = \mathrm{Tr}\left(T^N\right).} \tag{196}$$

The trace arises because we have imposed periodic boundary conditions. As T is a real symmetric matrix, it can be diagonalized, i.e.

$$U^\dagger T U = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}, \tag{197}$$

where U is a unitary matrix and

$$\lambda_\pm = e^{\beta J}\cosh(\beta h) \pm \sqrt{e^{2\beta J}\sinh^2(\beta h) + e^{-2\beta J}}. \tag{198}$$

Using the cyclicity of the trace and $UU^\dagger = I$, we have

$$Z = \mathrm{Tr}\left(UU^\dagger T^N\right) = \mathrm{Tr}\left(U^\dagger T^N U\right) = \mathrm{Tr}\left([U^\dagger T U]^N\right) = \mathrm{Tr}\begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} = \lambda_+^N + \lambda_-^N. \tag{199}$$

But as $\lambda_- < \lambda_+$ we have

$$Z = \lambda_+^N \left(1 + \left[\frac{\lambda_-}{\lambda_+}\right]^N\right) = \lambda_+^N \left(1 + e^{-N\ln(\lambda_+/\lambda_-)}\right). \tag{200}$$

So for large N, which is the case we are interested in, we have with exponential accuracy

$$\boxed{Z \simeq \lambda_+^N.} \tag{201}$$

Given the partition function, we can now easily calculate the magnetization per site

$$m(h) = \frac{1}{N\beta}\frac{\partial}{\partial h}\ln(Z). \tag{202}$$

In Fig. 7 we plot $m(h)$ as a function of inverse temperature $\beta = 1/k_B T$ for two values of magnetic field h. We see that for non-zero h, the magnetization per site takes its maximum value $m = 1$ at low temperatures. At high temperatures it goes to zero. This is as expected, as at low T the spins align along the direction of the applied field. However, as we decrease the field, the temperature below which $m(h)$ approaches unity decreases. In the limit $h \to 0$, the magnetization per site vanishes at all finite temperatures. Hence there is no phase transition to a ferromagnetically ordered state in the one dimensional Ising model.

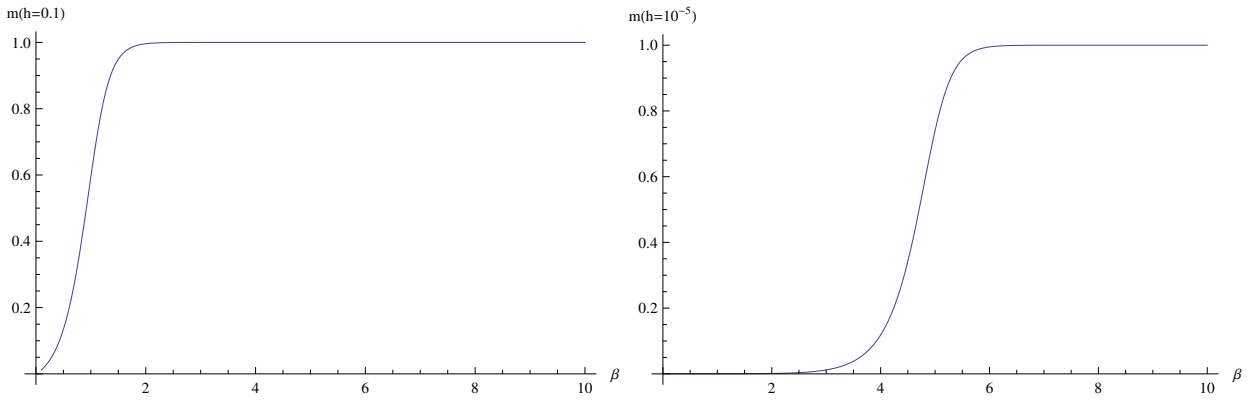


Figure 7: Magnetization per site as a function of inverse temperature for two values of applied magnetic field. We see that when we reduce the magnetic field, the temperature region in which the magnetization is essentially zero grows.

5.2.2 Averages of observables in the transfer matrix formalism

The average magnetization at site j is

$$\langle \sigma_j \rangle_\beta = \frac{1}{Z} \sum_{\sigma_1,\ldots,\sigma_N} \sigma_j e^{-\beta E(\{\sigma_j\})}. \tag{203}$$

We can express this in terms of the transfer matrix as

$$\langle \sigma_j \rangle_\beta = \frac{1}{Z} \sum_{\sigma_1,\ldots,\sigma_N} T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} \ldots T_{\sigma_{j-1}\sigma_j} \sigma_j T_{\sigma_j\sigma_{j+1}} \ldots T_{\sigma_N\sigma_1}. \tag{204}$$

Using that

$$\left(T\sigma^z\right)_{\sigma_{j-1}\sigma_j} = T_{\sigma_{j-1}\sigma_j}\sigma_j \ , \tag{205}$$

where $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is the Pauli matrix, we obtain

$$\langle \sigma_j \rangle_\beta = \frac{1}{Z} \mathrm{Tr}\left[T^{j-1}\sigma^z T^{N-j+1}\right] = \frac{1}{Z}\mathrm{Tr}\left[T^N \sigma^z\right]. \tag{206}$$

Diagonalizing T by means of a unitary transformation as before, this becomes

$$\langle \sigma_j \rangle_\beta = \frac{1}{Z}\mathrm{Tr}\left[U^\dagger T^N U U^\dagger \sigma^z U\right] = \frac{1}{Z}\mathrm{Tr}\left[\begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} U^\dagger \sigma^z U\right] \ . \tag{207}$$

The matrix U is given in terms of the normalized eigenvectors of T

$$T|\pm\rangle = \lambda_\pm |\pm\rangle \tag{208}$$

as

$$U = (|+\rangle, |-\rangle). \tag{209}$$

For $h = 0$ we have

$$U|_{h=0} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{210}$$

This gives

$$\langle \sigma_j \rangle_\beta \Big|_{h=0} = 0. \tag{211}$$

For general h the expression is more complicated

$$U = \begin{pmatrix} \frac{\alpha_+}{\sqrt{1+\alpha_+^2}} & \frac{\alpha_-}{\sqrt{1+\alpha_-^2}} \\ \frac{1}{\sqrt{1+\alpha_+^2}} & \frac{1}{\sqrt{1+\alpha_-^2}} \end{pmatrix} \quad , \quad \alpha_\pm = \sqrt{1+e^{4\beta J}\sinh^2(\beta h)} \pm e^{2\beta J}\sinh(\beta h). \tag{212}$$

The magnetization per site in the thermodynamic limit is then

$$\lim_{N\to\infty}\langle\sigma_j\rangle_\beta = \lim_{N\to\infty}\frac{\left(\frac{\alpha_+^2-1}{\alpha_+^2+1}\right)\lambda_+^N + \left(\frac{\alpha_-^2-1}{\alpha_-^2+1}\right)\lambda_-^N}{\lambda_+^N+\lambda_-^N} = \left(\frac{\alpha_+^2-1}{\alpha_+^2+1}\right). \tag{213}$$

This now allows us to prove, that in the one dimensional Ising model there is no phase transition at any finite temperature:

$$\boxed{\lim_{h\to 0}\lim_{N\to\infty}\langle\sigma_j\rangle_\beta = 0 \ , \quad \beta<\infty.} \tag{214}$$

Note the order of the limits here: we first take the infinite volume limit at finite h, and only afterwards take h to zero. This procedure allows for spontaneous symmetry breaking to occur, but the outcome of our calculation is that the spin reversal symmetry remains unbroken at any finite temperature.

Similarly, we find

$$\langle\sigma_j\sigma_{j+r}\rangle_\beta = \frac{1}{Z}\mathrm{Tr}\left[T^{j-1}\sigma^z T^r \sigma^z T^{N+1-j-r}\right] = \frac{1}{Z}\mathrm{Tr}\left[U^\dagger\sigma^z U\begin{pmatrix}\lambda_+^r & 0\\ 0 & \lambda_-^r\end{pmatrix}U^\dagger\sigma^z U\begin{pmatrix}\lambda_+^{N-r} & 0\\ 0 & \lambda_-^{N-r}\end{pmatrix}\right]. \tag{215}$$

We can evaluate this for zero field $h=0$

$$\langle\sigma_j\sigma_{j+r}\rangle_\beta\Big|_{h=0} = \frac{\lambda_+^{N-r}\lambda_-^r + \lambda_-^{N-r}\lambda_+^r}{\lambda_+^N+\lambda_-^N} \approx \left[\frac{\lambda_-}{\lambda_+}\right]^r = e^{-r/\xi}. \tag{216}$$

So in zero field the two-point function decays exponentially with *correlation length*

$$\xi = \frac{1}{\ln\coth(\beta J)}. \tag{217}$$

5.2.3 The related zero-dimensional quantum model

The 1D classical Ising model is related to a 0D quantum mechanical system as follows. Given the discussion leading to (181), we are looking to write the transfer matrix of the Ising model in the form

$$T = \sqrt{\frac{c}{\epsilon}}\, e^{-\epsilon H_Q/\hbar}, \tag{218}$$

where c is a constant with dimension of time. Our transfer matrix can be written as

$$T = e^{\beta J}\cosh(\beta h)I + e^{\beta J}\sinh(\beta h)\sigma^z + e^{-\beta J}\sigma^x \tag{219}$$

We see that if we tune h to zero such that for large β

$$e^{-2\beta J} = \frac{\epsilon K}{\hbar} \ , \quad \beta h e^{2\beta J} = \lambda = \text{fixed}, \tag{220}$$

then

$$T = \sqrt{\frac{\hbar}{\epsilon K}}\left(I + \frac{\epsilon K}{\hbar}\left[\lambda\sigma^z + \sigma^x\right] + \mathcal{O}(\epsilon^2)\right). \tag{221}$$

We conclude that the one dimensional classical Ising model is related to the quantum mechanics of a single spin-1/2 with Hamiltonian

$$H_Q = -K\sigma^x - K\lambda\sigma^z. \tag{222}$$

5.3 The Two-Dimensional Ising Model

We now turn to the 2D Ising model on a square lattice with periodic boundary conditions. The spin variables have now two indices corresponding to rows and columns of the square lattice respectively

$$\sigma_{j,k} = \pm 1 \ , \quad j,k = 1,\ldots,N. \tag{223}$$

The boundary conditions are $\sigma_{k,N+1} = \sigma_{k,1}$ and $\sigma_{N+1,j} = \sigma_{1,j}$, which correspond to the lattice "living" on

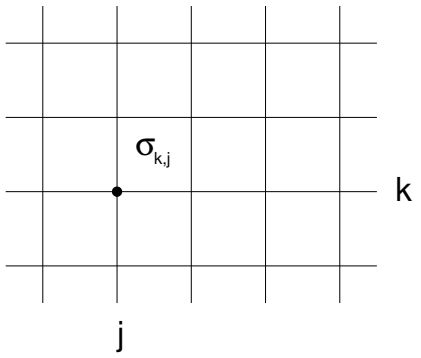


Figure 8: Ising model on the square lattice.

the surface of a torus. The energy in zero field is

$$E(\{\sigma_{k,j}\}) = -J \sum_{j,k} \sigma_{k,j}\sigma_{k,j+1} + \sigma_{k,j}\sigma_{k+1,j}. \tag{224}$$

5.3.1 Transfer Matrix Method

The partition function is given by

$$Z = \sum_{\{\sigma_{j,k}\}} e^{-\beta E(\{\sigma_{k,j}\})}. \tag{225}$$

The idea of the transfer matrix method is again to write this in terms of matrix multiplications. The difference to the one dimensional case is that the transfer matrix will now be much larger. We start by expressing the partition function in the form

$$Z = \sum_{\{\sigma_{j,k}\}} e^{-\beta \sum_{k=1}^{N} E(k;k+1)}, \tag{226}$$

where

$$E(k;k+1) = -J \sum_{j=1}^{N} \sigma_{k,j}\sigma_{k+1,j} + \frac{1}{2}\left[\sigma_{k,j}\sigma_{k,j+1} + \sigma_{k+1,j}\sigma_{k+1,j+1}\right]. \tag{227}$$

This energy depends only on the configurations of spins on rows k and $k+1$, i.e. on spins $\sigma_{k,1},\ldots,\sigma_{k,N}$ and $\sigma_{k+1,1},\ldots,\sigma_{k+1,N}$. Each configuration of spins on a given row specifies a sequence $s_1, s_2, \ldots, s_N$ with $s_j = \pm 1$. Let us associate a vector

$$|\boldsymbol{s}\rangle \tag{228}$$

with each such sequence. By construction there 2^N such vectors. We then define a scalar product on the space spanned by these vectors by

$$\langle \boldsymbol{t}|\boldsymbol{s}\rangle = \prod_{j=1}^{N} \delta_{t_j,s_j}. \tag{229}$$

With this definition, the vectors $\{|\boldsymbol{s}\rangle\}$ form an orthonormal basis of a 2^N dimensional linear vector space. In particular we have

$$I = \sum_{\boldsymbol{s}} |\boldsymbol{s}\rangle\langle\boldsymbol{s}|. \tag{230}$$

Finally, we define a $2^N \times 2^N$ *transfer matrix* T by

$$\langle\boldsymbol{\sigma}_k|T|\boldsymbol{\sigma}_{k+1}\rangle = e^{-\beta E(k;k+1)}. \tag{231}$$

The point of this construction is that the partition function can now be written in the form

$$Z = \sum_{\boldsymbol{\sigma}_1}\sum_{\boldsymbol{\sigma}_2}\cdots\sum_{\boldsymbol{\sigma}_N}\langle\boldsymbol{\sigma}_1|T|\boldsymbol{\sigma}_2\rangle\langle\boldsymbol{\sigma}_2|T|\boldsymbol{\sigma}_3\rangle\ldots\langle\boldsymbol{\sigma}_{N-1}|T|\boldsymbol{\sigma}_N\rangle\langle\boldsymbol{\sigma}_N|T|\boldsymbol{\sigma}_1\rangle \tag{232}$$

We now may use (230) to carry out the sums over spins, which gives

$$\boxed{Z = \mathrm{Tr}\left[T^N\right]}, \tag{233}$$

where the trace is over our basis $\{|\boldsymbol{s}\rangle|s_j = \pm 1\}$ of our 2^N dimensional vector space. Like in the 1D case, thermodynamic properties involve only the largest eigenvalues of T. Indeed, we have

$$Z = \sum_{j=1}^{2^N} \lambda_j^N \ , \tag{234}$$

where λ_j are the eigenvalues of T. The free energy is then

$$F = -k_B T \ln(Z) = -k_B T \ln\left[\lambda_{\max}^N \sum_{j=1}^{2^N}\left(\frac{\lambda_j}{\lambda_{\max}}\right)^N\right] = -k_B T N \ln(\lambda_{\max}) - k_B T \ln\left[\sum_j \left(\frac{\lambda_j}{\lambda_{\max}}\right)^N\right], \tag{235}$$

where $\lambda_{\max}$ is the largest eigenvalue of T, which we assume to be unique. As $|\lambda_j/\lambda_{\max}| < 1$, the second contribution in (235) is bounded by $-k_B T N \ln(2)$, and we see that in the thermodynamic limit the free energy per site is

$$\boxed{f = \lim_{N\to\infty}\frac{F}{N^2} = \lim_{N\to\infty} -\frac{k_B T}{N}\ln(\lambda_{\max}).} \tag{236}$$

Thermodynamic quantities are obtained by taking derivatives of f and hence only involve the largest eigenvalue of T. The main complication we have to deal with is that T is still a very large matrix. This poses the question, why we should bother to use a transfer matrix description anyway? Calculating Z from its basic definition (225) involves a sum with 2^{N^2} terms, i.e. at least 2^{N^2} operations on a computer. Finding the largest eigenvalue of a $M \times M$ matrix involves $\mathcal{O}(M^2)$ operations, which in our case amounts to $\mathcal{O}(2^{2N})$. For large values of N this amounts to an enormous simplification.

5.3.2 Spontaneous Symmetry Breaking

Surprisingly, the transfer matrix of the 2D Ising model can be diagonalized exactly. Unfortunately we don't have the time do go through the somewhat complicated procedure here, but the upshot is that the 2D Ising model can be solved *exactly*. Perhaps the most important result is that in the thermodynamic limit the square lattice Ising model has a *finite temperature phase transition* between a paramagnetic and a ferromagnetic phase. The magnetization per site behaves as shown in Fig.9. At low temperatures $T < T_c$ there is a non-zero magnetization per site, even though we did not apply a magnetic field. This is surprising, because our energy (224) is unchanged if we flip all spins

$$\sigma_{j,k} \to -\sigma_{j,k}. \tag{237}$$

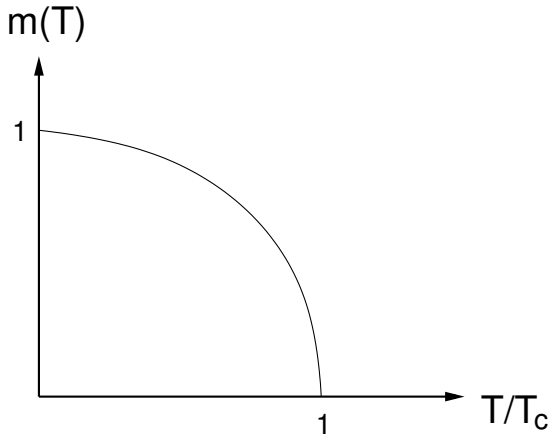


Figure 9: Phase Transition in the square lattice Ising model.

The operation (237) is a discrete (two-fold) symmetry of the Ising model. Because we have translational invariance, the magnetization per site is

$$m = \langle \sigma_{j,k} \rangle_\beta. \tag{238}$$

Hence a non-zero value of m signifies the *spontaneous breaking* of the discrete symmetry (237). In order to describe this effect mathematically, we have to invoke a bit of trickery. Let us consider zero temperature. Then there are exactly two degenerate lowest energy states: the one with all spins $\sigma_{j,k} = +1$ and the one with all spins $\sigma_{j,k} = -1$. We now apply a very small magnetic field to the system, i.e. add a term

$$\delta E = -\epsilon \sum_{j,k} \sigma_{j,k} \tag{239}$$

to the energy. This splits the two states, which now have energies

$$E_\pm = -JN_B \mp \epsilon N \ , \tag{240}$$

where N_B is the number of bonds. The next step is key: we now *define* the thermodynamic limit of the free energy per site as

$$f(T) \equiv \lim_{\epsilon \to 0} \lim_{N \to \infty} \frac{-k_B T \ln(Z)}{N^2}. \tag{241}$$

The point is that the contributions $Z_\pm = e^{-\beta E_\pm}$ of the two states to Z are such that

$$\frac{Z_-}{Z_+} = e^{-2\epsilon N/k_B T} \ . \tag{242}$$

This goes to zero when we take N to infinity! So in the above sequence of limits, only the state with all spins up contributes to the partition function, and this provides a way of describing spontaneous symmetry breaking! The key to this procedure is that

$$\boxed{\lim_{\epsilon \to 0} \lim_{N \to \infty} Z \neq \lim_{N \to \infty} \lim_{\epsilon \to 0} Z.} \tag{243}$$

The procedure we have outlined above, i.e. introducing a symmetry breaking field, then taking the infinite volume limit, and finally removing the field, is very general and applies to all instances where spontaneous symmetry breaking occurs.

5.4 Homework Questions 8-10

Question 8. A lattice model for non-ideal gas is defined as follows. The sites i of a lattice may be empty or occupied by at most one atom, and the variable n_i takes the values $n_i = 0$ and $n_i = 1$ in the two cases. There is an attractive interaction energy J between atoms that occupy neighbouring sites, and a chemical potential μ. The model Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle ij \rangle} n_i n_j - \mu \sum_i n_i \,, \tag{244}$$

where $\sum_{\langle ij \rangle}$ is a sum over neighbouring pairs of sites.
(a) Describe briefly how the *transfer matrix method* may be used to calculate the statistical-mechanical properties of one-dimensional lattice models with short range interactions. Illustrate your answer by explaining how the partition function for a one-dimensional version of the lattice gas, Eq. (1), defined on a lattice of N sites with periodic boundary conditions, may be evaluated using the matrix

$$\mathbf{T} = \begin{pmatrix} 1 & \mathrm{e}^{\beta\mu/2} \\ \mathrm{e}^{\beta\mu/2} & \mathrm{e}^{\beta(J+\mu)} \end{pmatrix} .$$

(b) Derive an expression for $\langle n_i \rangle$ in the limit $N \to \infty$, in terms of elements of the eigenvectors of this matrix.
(c) Show that

$$\langle n_i \rangle = \frac{1}{1 + \mathrm{e}^{-2\theta}} \,,$$

where

$$\sinh(\theta) = \exp(\beta J/2) \sinh(\beta[J+\mu]/2) \,.$$

Sketch $\langle n_i \rangle$ as a function of μ for $\beta J \gg 1$, and comment on the physical significance of your result.

Question 9. The one-dimensional 3-state Potts model is defined as follows. At lattice sites $i = 0, 1, \ldots, L$ "spin" variables σ_i take integer values $\sigma_i = 1, 2, 3$. The Hamiltonian is then given by

$$H = -J \sum_{i=0}^{L-1} \delta_{\sigma_i, \sigma_{i+1}} , \tag{245}$$

where $\delta_{a,b}$ is the Kronecker delta, $J > 0$.
(a) What are the ground states and first excited states for this model?
(b) Write down the transfer matrix for (245). Derive an expression for the free energy per site f in the limit of large L in terms of the transfer matrix eigenvalues. Show that vectors of the form $(1, z, z^2)$ with $z^3 = 1$ are eigenvectors, and hence find the corresponding eigenvalues. Show that at temperature T (with $\beta = 1/k_B T$) and in the limit $L \to \infty$

$$f = -k_B T \ln \left(3 + e^{\beta J} - 1 \right) . \tag{246}$$

(c) The boundary variable σ_0 is fixed in the state $\sigma_0 = 1$. Derive an expression (for large L), that the variable at site $\ell \gg 1$ is in the same state, in terms of the transfer matrix eigenvalues and eigenvectors. Show that your result has the form

$$\langle \delta_{\sigma_\ell, 1} \rangle = \frac{1}{3} + \frac{2}{3} e^{-\ell/\xi} . \tag{247}$$

How does ξ behave in the low and high temperature limits?

Question 10. Consider a one dimensional Ising model on an open chain with N sites, where N is odd. On all even sites a magnetic field $2h$ is applied, see Fig. 10. The energy is

$$E = -J \sum_{j=1}^{N-1} \sigma_j \sigma_{j+1} + 2h \sum_{j=1}^{(N-1)/2} \sigma_{2j} . \tag{248}$$

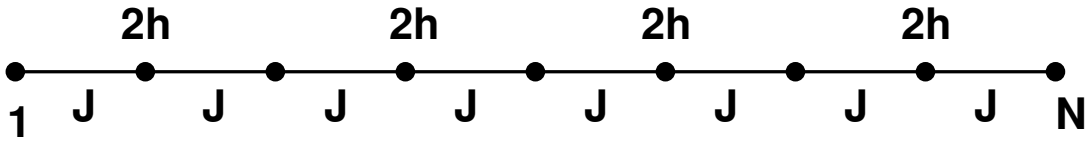


Figure 10: Open Ising chain with magnetic field applied to all even sites.

(a) Show that the partition function can be written in the form

$$Z = \langle u|T^{(N-1)/2}|v\rangle \ , \tag{249}$$

where T is an appropriately constructed transfer matrix, and $|u\rangle$ and $|v\rangle$ two dimensional vectors. Give explicit expressions for T, $|u\rangle$ and $|v\rangle$.
(b) Calculate Z for the case $h = 0$.

Part III
Many-Particle Quantum Mechanics

In the basic QM course you encountered only quantum systems with *very small numbers* of particles. In the harmonic oscillator problem we are dealing with a single QM particle, when solving the hydrogen atom we had one electron and one nucleus. Perhaps the most important field of application of quantum physics is to systems of *many* particles. Examples are the electronic degrees of freedom in solids, superconductors, trapped ultra-cold atomic gases, magnets and so on. The methods you have encountered in the basic QM course are not suitable for studying such problems. In this part of the course we introduce a framework, that will allow us to study the QM of many-particle systems. This new way of looking at things will also reveal very interesting connections to *Quantum Field Theory*.

6 Second Quantization

The formalism we develop in the following is known as *second quantization*.

6.1 Systems of Independent Particles

You already know from second year QM how to solve problems involving *independent particles*

$$H = \sum_{j=1}^{N} H_j \tag{250}$$

where H_j is the Hamiltonian on the j'th particle, e.g.

$$H_j = \frac{\hat{\mathbf{p}}_j^2}{2m} + V(\hat{\mathbf{r}}_j) = -\frac{\hbar^2}{2m}\nabla_j^2 + V(\hat{\mathbf{r}}_j). \tag{251}$$

The key to solving such problems is that $[H_j, H_l] = 0$. We'll now briefly review the necessary steps, switching back and forth quite freely between using states and operators acting on them, and the position representation of the problem (i.e. looking at wave functions).

- Step 1. Solve the single-particle problem

$$H_j|\phi_l\rangle = E_l|\phi_l\rangle \ . \tag{252}$$

  The corresponding wave functions are

$$\phi_l(\mathbf{r}_j) = \langle \mathbf{r}_j|\phi_l\rangle. \tag{253}$$

  The eigenstates form an orthonormal set

$$\langle\phi_l|\phi_m\rangle = \delta_{l,m} = \int d^D\mathbf{r}_j \ \phi_l^*(\mathbf{r}_j)\phi_m(\mathbf{r}_j). \tag{254}$$

- Step 2. Form N-particle eigenfunctions as *products*

$$\left(\sum_{j=1}^{N} H_j\right) \phi_{l_1}(\mathbf{r}_1)\phi_{l_2}(\mathbf{r}_2)\dots\phi_{l_N}(\mathbf{r}_N) = \left(\sum_{j=1}^{N} E_{l_j}\right) \phi_{l_1}(\mathbf{r}_1)\phi_{l_2}(\mathbf{r}_2)\dots\phi_{l_N}(\mathbf{r}_N) \ . \tag{255}$$

  This follows from the fact that in the position representation H_j is a differential operator that acts only on the j'th position $\mathbf{r}_j$. The corresponding eigenstates are tensor products

$$|l_1\rangle \otimes |l_2\rangle \otimes \cdots \otimes |l_N\rangle. \tag{256}$$

- Step 3. Impose the appropriate *exchange symmetry* for indistinguishable particles, e.g.

$$\psi_{\pm}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \left[\phi_l(\mathbf{r}_1)\phi_m(\mathbf{r}_2) \pm \phi_l(\mathbf{r}_2)\phi_m(\mathbf{r}_1)\right] \ , \quad l \neq m. \tag{257}$$

Generally we require

$$\psi(\dots, \mathbf{r}_i, \dots, \mathbf{r}_j, \dots) = \pm\psi(\dots, \mathbf{r}_j, \dots, \mathbf{r}_i, \dots) \ , \tag{258}$$

where the + sign corresponds to bosons and the − sign to fermions. This is achieved by taking

$$\boxed{\psi_{l_1 \dots l_N}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \mathcal{N} \sum_{P \in S_N} (\pm 1)^{|P|} \phi_{l_{P_1}}(\mathbf{r}_1) \dots \phi_{l_{P_N}}(\mathbf{r}_N),} \tag{259}$$

where the sum is over all permutations of $(1, 2, \dots, N)$ and $|P|$ is the number of pair exchanges required to reduce $(P_1, \dots, P_N)$ to $(1, \dots, N)$. The normalization constant $\mathcal{N}$ is

$$\mathcal{N} = \frac{1}{\sqrt{N! n_1! n_2! \dots}} \ , \tag{260}$$

where n_j is the number of times j occurs in the set $\{l_1, \dots, l_N\}$. For fermions the wave functions can be written as *Slater determinants*

$$\psi_{l_1 \dots l_N}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \phi_{l_1}(\mathbf{r}_1) & \dots & \phi_{l_1}(\mathbf{r}_N) \\ \vdots & & \vdots \\ \phi_{l_N}(\mathbf{r}_1) & \dots & \phi_{l_N}(\mathbf{r}_N) \end{pmatrix} . \tag{261}$$

The states corresponding to (259) are

$$\boxed{|l_1, \dots, l_N\rangle = \mathcal{N} \sum_{P \in S_N} (\pm 1)^{|P|} |l_{P_1}\rangle \otimes \dots \otimes |l_{P_N}\rangle \ .} \tag{262}$$

6.1.1 Occupation Number Representation

By construction the states have the symmetry

$$|l_{Q_1} \dots l_{Q_N}\rangle = \pm |l_1 \dots l_N\rangle \ , \tag{263}$$

where Q is an arbitrary permutation of $(1, \dots, N)$. As the overall sign of state is irrelevant, we can therefore choose them without loss of generality as

$$|\underbrace{1 \dots 1}_{n_1} \underbrace{2 \dots 2}_{n_2} \underbrace{3 \dots 3}_{n_3} 4 \dots\rangle \equiv |n_1 n_2 n_3 \dots\rangle. \tag{264}$$

In (264) we have as many n_j's as there are single-particle eigenstates, i.e. $\dim H$ [4]. For fermions we have $n_j = 0, 1$ only as a consequence of the *Pauli principle*. The representation (264) is called *occupation number representation*. The n_j's tell us how many particles are in the single-particle state $|j\rangle$. By construction the states $\{|n_1 n_2 n_3 \dots\rangle | \sum_j n_j = N\}$ form an orthonormal basis of our N-particle problem

$$\langle m_1 m_2 m_3 \dots | n_1 n_2 n_3 \dots \rangle = \prod_j \delta_{n_j, m_j} \ , \tag{265}$$

where we have defined $\langle m_1 m_2 m_3 \dots | = | m_1 m_2 m_3 \dots \rangle^\dagger$.

[4] Note that this is different from the particle number N.

6.2 Fock Space

We now want to allow the particle number to vary. The main reason for doing this is that we will encounter physical problems where particle number is in fact not conserved. Another motivation is that experimental probes like photoemission change particle number, and we want to be able to describe these. The resulting space of states is called *Fock Space*.

1. The state with no particles is called the *vacuum state* and is denoted by $|0\rangle$.
2. N-particle states are $|n_1 n_2 n_3 \dots\rangle$ with $\sum_j n_j = N$.

6.2.1 Creation and Annihilation Operators

Given a basis of our space of states we can define operators by specifying their action on all basis states.

- particle creation operators with quantum number l

$$\boxed{c_l^\dagger |n_1 n_2 \dots\rangle = \begin{cases} 0 & \text{if } n_l = 1 \text{ for fermions} \\ \sqrt{n_l+1}(\pm 1)^{\sum_{j=1}^{l-1} n_j} |n_1 n_2 \dots n_l + 1 \dots\rangle & \text{else.} \end{cases}} \tag{266}$$

  Here the $+$ $(-)$ sign applies to bosons (fermions).

- particle annihilation operators with quantum number l

$$\boxed{c_l |n_1 n_2 \dots\rangle = \sqrt{n_l}(\pm 1)^{\sum_{j=1}^{l-1} n_j} |n_1 n_2 \dots n_l - 1 \dots\rangle \ .} \tag{267}$$

We note that (267) follows from (266) by

$$\langle m_1 m_2 \dots | c_l^\dagger | n_1 n_2 \dots\rangle^* = \langle n_1 n_2 \dots | c_l | m_1 m_2 \dots\rangle \ . \tag{268}$$

The creation and annihilation operators fulfil *canonical (anti)commutation relations*

$$\boxed{[c_l, c_m] = 0 = [c_l^\dagger, c_m^\dagger] \ , \quad [c_l, c_m^\dagger] = \delta_{l,m} \qquad \text{bosons,}} \tag{269}$$

$$\boxed{\{c_l, c_m\} = c_l c_m + c_m c_l = 0 = \{c_l^\dagger, c_m^\dagger\} \ , \quad \{c_l, c_m^\dagger\} = \delta_{l,m} \qquad \text{fermions.}} \tag{270}$$

Proof

Let us see how to prove these in the fermionic case. For $l < m$ we have

$$\begin{aligned} c_l^\dagger c_m |\dots n_l \dots n_m \dots\rangle &= c_l^\dagger \sqrt{n_m}(-1)^{\sum_{j=1}^{m-1} n_j} |\dots n_l \dots n_m - 1 \dots\rangle \\ &= \sqrt{n_l+1}\sqrt{n_m}(-1)^{\sum_{j=l}^{m-1} n_j} |\dots n_l + 1 \dots n_m - 1 \dots\rangle. \end{aligned} \tag{271}$$

Similarly we have

$$c_m c_l^\dagger |\dots n_l \dots n_m \dots\rangle = \sqrt{n_l+1}\sqrt{n_m}(-1)^{1+\sum_{j=l}^{m-1} n_j} |\dots n_l + 1 \dots n_m - 1 \dots\rangle. \tag{272}$$

This means that for any basis state $|n_1 n_2 \dots\rangle$ we have

$$\{c_l^\dagger, c_m\} |n_1 n_2 \dots\rangle = 0 \ , \qquad \text{if } l > m. \tag{273}$$

This implies that

$$\{c_l^\dagger, c_m\} = 0 \ , \qquad \text{if } l > m. \tag{274}$$

The case $l < m$ works in the same way. This leaves us with the case $l = m$. Here we have

$$c_l^\dagger c_l |\dots n_l \dots n_m \dots\rangle = c_l^\dagger \sqrt{n_l}(-1)^{\sum_{j=1}^{l-1} n_j} |\dots n_l - 1 \dots\rangle = n_l |\dots n_l \dots\rangle. \tag{275}$$

$$\begin{aligned} c_l c_l^\dagger |\dots n_l \dots\rangle &= \begin{cases} c_l \sqrt{n_l + 1}(-1)^{\sum_{j=1}^{l-1} n_j} |\dots n_l + 1 \dots\rangle & \text{if } n_l = 0 \ , \\ 0 & \text{if } n_l = 1 \ , \end{cases} \\ &= \begin{cases} |\dots n_l \dots\rangle & \text{if } n_l = 0 \ , \\ 0 & \text{if } n_l = 1 \ , \end{cases} \end{aligned} \tag{276}$$

Combining these we find that

$$\{c_l^\dagger, c_l\} |\dots n_l \dots\rangle = |\dots n_l \dots\rangle \ , \tag{277}$$

and as the states $|\dots n_l \dots\rangle$ form a basis this implies

$$\{c_l^\dagger, c_l\} = 1. \tag{278}$$

Note that here 1 really means the identity operator $\mathbf{1}$.

PROOF

6.2.2 Basis of the Fock Space

We are now in a position to write down our Fock space basis in a very convenient way.

- Fock vacuum (state without any particles)
$$|0\rangle. \tag{279}$$
- Single-particle states
$$|0 \dots 0 \underbrace{1}_{l} 0 \dots\rangle = c_l^\dagger |0\rangle \ . \tag{280}$$
- N-particle states
$$|n_1 n_2 \dots\rangle = \prod_j \frac{1}{\sqrt{n_j!}} \left(c_j^\dagger\right)^{n_j} |0\rangle \ . \tag{281}$$

6.3 Homework Questions 11-13

Question 11. Consider a fermion 'system' with just one single-particle orbital, so that the only states of the system are $|0\rangle$ (unoccupied) and $|1\rangle$ (occupied). Show that we can represent the operators a and $a^\dagger$ by the matrices

$$a^\dagger = \begin{pmatrix} 0 & 0 \\ C & 0 \end{pmatrix}, \quad a = \begin{pmatrix} 0 & C^* \\ 0 & 0 \end{pmatrix}.$$

You can do this by checking the values of aa, $a^\dagger a^\dagger$ and $a^\dagger a + a a^\dagger$. What values may the constant C take?

Question 12. A quantum-mechanical Hamiltonian for a system of an even number N of point unit masses interacting by nearest-neighbour forces in one dimension is given by

$$H = \frac{1}{2} \sum_{r=1}^{N} \left(p_r^2 + (q_{r+1} - q_r)^2\right),$$

where the Hermitian operators q_r, p_r satisfy the commutation relations $[q_r, q_s] = [p_r, p_s] = 0$, $[q_r, p_s] = \mathrm{i}\delta_{rs}$, and where $q_{r+N} = q_r$. New operators Q_k, P_k are defined by

$$q_r = \frac{1}{\sqrt{N}} \sum_k Q_k \mathrm{e}^{\mathrm{i}kr} \qquad \text{and} \qquad p_r = \frac{1}{\sqrt{N}} \sum_k P_k \mathrm{e}^{-\mathrm{i}kr},$$

where $k = 2\pi n/N$ with $n = -N/2 + 1, \ldots, 0, \ldots, N/2$.

Show that:

(a) $Q_k = \dfrac{1}{\sqrt{N}} \displaystyle\sum_{s=1}^{N} q_s \mathrm{e}^{-\mathrm{i}ks}$ and $P_k = \frac{1}{\sqrt{N}} \sum_{s=1}^{N} p_s \mathrm{e}^{\mathrm{i}ks}$

(b) $[Q_k, P_{k'}] = \mathrm{i}\delta_{kk'}$

(c) $H = \frac{1}{2}\Big(\sum_k P_k P_{-k} + \omega^2 Q_k Q_{-k} \Big)$, where $\omega^2 = 2(1 - \cos k)$.

Similarly to the treatment of the simple harmonic oscillator in QM I we then define annihilation operators a_k by

$$a_k = \frac{1}{(2\omega_k)^{1/2}} (\omega_k Q_k + \mathrm{i} P_{-k}).$$

Show that the Hermitian conjugate operators are

$$a_k^\dagger = \frac{1}{(2\omega_k)^{1/2}} (\omega_k Q_{-k} - \mathrm{i} P_k),$$

and determine the canonical commutation relations for a_k and $a_p^\dagger$. Construct the Fock space of states and determine the eigenstates and eigenvalues of H.

Question 13. Bosonic creation operators are defined through their action on basis states in the occupation number representation as

$$c_l^\dagger |n_1 n_2 \ldots\rangle = \sqrt{n_l + 1} |n_1 n_2 \ldots n_l + 1 \ldots\rangle \ , \tag{282}$$

a) Deduce from this how bosonic annihilation operators act.
b) Show that the creation and annihilation operators fulfil *canonical commutation relations*

$$[c_l, c_m] = 0 = [c_l^\dagger, c_m^\dagger] \ , \quad [c_l, c_m^\dagger] = \delta_{l,m}. \tag{283}$$

6.3.1 Change of Basis

The Fock space is built from a given basis of single-particle states

$$\boxed{\text{single-particle states } |l\rangle} \longrightarrow \boxed{\text{N-particle states } |n_1 n_2 \ldots\rangle} \longrightarrow \boxed{\text{Fock Space}}. \tag{284}$$

You know from second year QM that it is often convenient to switch from one basis to another, e.g. from energy to momentum eigenstates. This is achieved by a unitary transformation

$$\{|l\rangle\} \longrightarrow \{|\alpha\rangle\} \ , \tag{285}$$

where

$$|\alpha\rangle = \sum_l \underbrace{\langle l|\alpha\rangle}_{U_{l\alpha}} |l\rangle. \tag{286}$$

By construction

$$\sum_\alpha U_{l\alpha} U_{\alpha m}^\dagger = \sum_\alpha \langle l|\alpha\rangle\langle\alpha|m\rangle = \langle l|m\rangle = \delta_{lm}. \tag{287}$$

We now want to "lift" this unitary transformation to the level of the Fock space. We know that

$$\begin{aligned} |l\rangle &= c_l^\dagger|0\rangle \ , \\ |\alpha\rangle &= d_\alpha^\dagger|0\rangle \ . \end{aligned} \tag{288}$$

On the other hand we have

$$|\alpha\rangle = \sum_l U_{l\alpha}|l\rangle = \sum_l U_{l\alpha}c_l^\dagger|0\rangle. \tag{289}$$

This suggests that we take

$$\boxed{d_\alpha^\dagger = \sum_l U_{l\alpha}c_l^\dagger,} \tag{290}$$

and this indeed reproduces the correct transformation for N-particle states. Taking the hermitian conjugate we obtain the transformation law for annihilation operators

$$\boxed{d_\alpha = \sum_l U_{\alpha l}^\dagger c_l.} \tag{291}$$

We emphasize that these transformation properties are compatible with the (anti)commutation relations (as they must be). For fermions

$$\{d_\alpha, d_\beta^\dagger\} = \sum_{l,m} U_{\alpha l}^\dagger U_{m\beta} \underbrace{\{c_l, c_m^\dagger\}}_{\delta_{l,m}} = \sum_l U_{\alpha l}^\dagger U_{l\beta} = (U^\dagger U)_{\alpha\beta} = \delta_{\alpha,\beta}. \tag{292}$$

6.4 Second Quantized Form of Operators

In the next step we want to know how observables such as H, P, X etc act on the Fock space.

6.4.1 Occupation number operators

These are the simplest hermitian operators we can build from c_l and $c_m^\dagger$. They are defined as

$$\hat{n}_l \equiv c_l^\dagger c_l. \tag{293}$$

From the definition of c_l and $c_l^\dagger$ it follows immediately that

$$\hat{n}_l|n_1 n_2 \dots\rangle = n_l|n_1 n_2 \dots\rangle. \tag{294}$$

6.4.2 Single-particle operators

Single-particle operators are of the form

$$\hat{O} = \sum_j \hat{o}_j \ , \tag{295}$$

where the operator $\hat{o}_j$ acts only on the j'th particle. Examples are kinetic and potential energy operators

$$\hat{T} = \sum_j \frac{\hat{p}_j^2}{2m} \ , \qquad \hat{V} = \sum_j V(\hat{x}_j). \tag{296}$$

We want to represent $\hat{O}$ on the Fock space built from single-particle eigenstates $|\alpha\rangle$. We do this in two steps:

- Step 1: We first represent $\hat{O}$ on the Fock space built from the eigenstates of $\hat{o}$

$$\hat{o}|l\rangle = \lambda_l |l\rangle = \lambda_l c_l^\dagger |0\rangle. \tag{297}$$

Then, when acting on an N-particle state (262), we have

$$\hat{O}|l_1, l_2, \ldots, l_N\rangle = \left[\sum_{j=1}^{N} \lambda_j\right] |l_1, l_2, \ldots, l_N\rangle. \tag{298}$$

This is readily translated into the occupation number representation

$$\hat{O}|n_1 n_2 \ldots\rangle = \left[\sum_k n_k \lambda_k\right] |n_1 n_2 \ldots\rangle. \tag{299}$$

As $|n_1 n_2 \ldots\rangle$ constitute a basis, this together with (294) imply that we can represent $\hat{O}$ in the form

$$\hat{O} = \sum_k \lambda_k \hat{n}_k = \sum_k \lambda_k c_k^\dagger c_k. \tag{300}$$

- Step 2: Now that we have a representation of $\hat{O}$ on the Fock space built from the single-particle states $|l\rangle$, we can use a basis transformation to the basis $\{|\alpha\rangle\}$ to obtain a representation on a general Fock space. Using that $\langle k|\hat{O}|k'\rangle = \delta_{k,k'}\lambda_k$ we can rewrite (300) in the form

$$\hat{O} = \sum_{k,k'} \langle k'|\hat{O}|k\rangle c_{k'}^\dagger c_k. \tag{301}$$

Then we apply our general rules for a change of single-particle basis of the Fock space

$$c_k^\dagger = \sum_\alpha U_{\alpha k}^\dagger d_\alpha^\dagger. \tag{302}$$

This gives

$$\hat{O} = \sum_{\alpha,\beta} \underbrace{\sum_{k'} \left(\langle k'|U_{\alpha k'}^\dagger\right)}_{\langle\alpha|} \hat{O} \underbrace{\sum_k \left(U_{k\beta}|k\rangle\right)}_{|\beta\rangle} d_\alpha^\dagger d_\beta. \tag{303}$$

where we have used that

$$|k\rangle = \sum_\alpha U_{\alpha k}^\dagger |\alpha\rangle \ . \tag{304}$$

This gives us the final result

$$\boxed{\hat{O} = \sum_{\alpha,\beta} \langle\alpha|\hat{O}|\beta\rangle \ d_\alpha^\dagger d_\beta.} \tag{305}$$

We now work out a number of explicit examples of Fock space representations for single-particle operators.

1. Momentum Operators $\mathbf{P}$ in the infinite volume:

(i) Let us first consider $\mathbf{P}$ in the single-particle basis of momentum eigenstates

$$\hat{\mathbf{P}}|\mathbf{k}\rangle = \mathbf{k}|\mathbf{k}\rangle \ , \quad \langle\mathbf{p}|\mathbf{k}\rangle = (2\pi\hbar)^3 \delta^{(3)}(\mathbf{p} - \mathbf{k}). \tag{306}$$

REMARK

These are shorthand notations for

$$\hat{P}_a|k_x,k_y,k_z\rangle = k_a|k_x,k_y,k_z\rangle \ , \quad a=x,y,z. \tag{307}$$

and

$$\langle p_x,p_y,p_z|k_x,k_y,k_z\rangle = (2\pi\hbar)^3\delta(k_x-p_x)\delta(k_y-p_y)\delta(k_z-p_z) \ . \tag{308}$$

REMARK

Using our general result for representing single-particle operators in a Fock space built from their eigenstates (300) we have

$$\hat{\mathbf{P}} = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\mathbf{p}c^\dagger(\mathbf{p})c(\mathbf{p}) \ , \qquad [c^\dagger(\mathbf{k}),c(\mathbf{p})\} = (2\pi\hbar)^3\delta^{(3)}(\mathbf{p}-\mathbf{k}). \tag{309}$$

Here we have introduced a notation

$$[c^\dagger(\mathbf{k}),c(\mathbf{p})\} = \begin{cases} c^\dagger(\mathbf{k})c(\mathbf{p}) - c(\mathbf{p})c^\dagger(\mathbf{k}) & \text{for bosons} \\ c^\dagger(\mathbf{k})c(\mathbf{p}) + c(\mathbf{p})c^\dagger(\mathbf{k}) & \text{for fermions.} \end{cases} \tag{310}$$

(ii) Next we want to represent $\hat{\mathbf{P}}$ in the single-particle basis of position eigenstates

$$\hat{\mathbf{X}}|\mathbf{x}\rangle = \mathbf{x}|\mathbf{x}\rangle \ , \quad \langle\mathbf{x}|\mathbf{x}'\rangle = \delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{311}$$

Our general formula (305) gives

$$\hat{\mathbf{P}} = \int d^3\mathbf{x}d^3\mathbf{x}' \ \langle\mathbf{x}'|\hat{\mathbf{P}}|\mathbf{x}\rangle c^\dagger(\mathbf{x}')c(\mathbf{x}) \ . \tag{312}$$

We can simplify this by noting that

$$\langle\mathbf{x}'|\hat{\mathbf{P}}|\mathbf{x}\rangle = -i\hbar\nabla_{\mathbf{x}'}\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{313}$$

which allows us to eliminate three of the integrals

$$\hat{\mathbf{P}} = \int d^3\mathbf{x}d^3\mathbf{x}' \left[-i\hbar\nabla_{\mathbf{x}'}\delta^{(3)}(\mathbf{x}-\mathbf{x}')\right] c^\dagger(\mathbf{x}')c(\mathbf{x}) = \int d^3\mathbf{x}c^\dagger(\mathbf{x})\left(-i\hbar\nabla_{\mathbf{x}}\right)c(\mathbf{x}). \tag{314}$$

2. Single-particle Hamiltonian:

$$H = \sum_{j=1}^{N}\frac{\hat{\mathbf{p}}_j^2}{2m} + V(\hat{\mathbf{x}}_j). \tag{315}$$

(i) Let us first consider H in the single-particle basis of energy eigenstates $H|l\rangle = E_l|l\rangle$, $|l\rangle = c_l^\dagger|0\rangle$. Our result (300) tells us that

$$H = \sum_l E_l c_l^\dagger c_l. \tag{316}$$

(ii) Next we consider the position representation, i.e. we take position eigenstates $|\mathbf{x}\rangle = c^\dagger(\mathbf{x})|0\rangle$ as a basis of single-particle states. Then by (305)

$$H = \int d^3\mathbf{x}d^3\mathbf{x}' \ \langle\mathbf{x}'|H|\mathbf{x}\rangle \ c^\dagger(\mathbf{x}')c(\mathbf{x}). \tag{317}$$

Substituting (315) into (317) and using

$$\langle\mathbf{x}'|V(\hat{\mathbf{x}})|\mathbf{x}\rangle = V(\mathbf{x})\delta^{(3)}(\mathbf{x}-\mathbf{x}') \ , \quad \langle\mathbf{x}'|\hat{\mathbf{p}}^2|\mathbf{x}\rangle = -\hbar^2\nabla^2\delta^{(3)}(\mathbf{x}-\mathbf{x}') \ , \tag{318}$$

we arrive at the position representation

$$\boxed{H = \int d^3\mathbf{x}\; c^\dagger(\mathbf{x}) \left[-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{x}) \right] c(\mathbf{x}).} \tag{319}$$

(iii) Finally we consider the momentum representation, i.e. we take momentum eigenstates $|\mathbf{p}\rangle = c^\dagger(\mathbf{p})|0\rangle$ as a basis of single-particle states. Then by (305)

$$H = \int \frac{d^3\mathbf{p} d^3\mathbf{p}'}{(2\pi\hbar)^6}\; \langle \mathbf{p}'|H|\mathbf{p}\rangle\; c^\dagger(\mathbf{p}')c(\mathbf{p}). \tag{320}$$

Matrix elements of the kinetic energy operator are simple

$$\langle \mathbf{p}'|\hat{\mathbf{p}}^2|\mathbf{p}\rangle = \mathbf{p}^2\langle \mathbf{p}'|\mathbf{p}\rangle = \mathbf{p}^2(2\pi\hbar)^3\delta^{(3)}(\mathbf{p}-\mathbf{p}'). \tag{321}$$

Matrix elements of the potential can be calcuated as follows

$$\begin{aligned} \langle \mathbf{p}'|\hat{V}|\mathbf{p}\rangle &= \int d^3\mathbf{x} d^3\mathbf{x}'\; \langle \mathbf{p}'|\mathbf{x}'\rangle\langle \mathbf{x}'|\hat{V}|\mathbf{x}\rangle\langle \mathbf{x}|\mathbf{p}\rangle = \int d^3\mathbf{x} d^3\mathbf{x}' \quad \underbrace{\langle \mathbf{x}'|\hat{V}|\mathbf{x}\rangle}_{V(\mathbf{x})\delta^{(3)}(\mathbf{x}-\mathbf{x}')} \quad e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x} - \frac{i}{\hbar}\mathbf{p}'\cdot\mathbf{x}'} \\ &= \int d^3\mathbf{x}\; V(\mathbf{x}) e^{\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{x}} = \tilde{V}(\mathbf{p}-\mathbf{p}'), \end{aligned} \tag{322}$$

where $\tilde{V}(\mathbf{p})$ is essentially the *three-dimensional Fourier transform* of the (ordinary) function $V(\mathbf{x})$. Hence

$$\boxed{H = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\; \frac{\mathbf{p}^2}{2m} c^\dagger(\mathbf{p})c(\mathbf{p}) + \int \frac{d^3\mathbf{p} d^3\mathbf{p}'}{(2\pi\hbar)^6}\; \tilde{V}(\mathbf{p}-\mathbf{p}')c^\dagger(\mathbf{p}')c(\mathbf{p}).} \tag{323}$$

6.4.3 Two-particle operators

These are operators that act on two particles at a time. A good example is the interaction potential $V(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)$ between two particles at positions $\mathbf{r}_1$ and $\mathbf{r}_2$. For N particles we want to consider

$$\hat{V} = \sum_{i<j}^{N} V(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j). \tag{324}$$

On the Fock space built from single-particle position eigenstates this is represented as

$$\boxed{\hat{V} = \frac{1}{2}\int d^3\mathbf{r} d^3\mathbf{r}'\; c^\dagger(\mathbf{r})c^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')c(\mathbf{r}')c(\mathbf{r}).} \tag{325}$$

Note that when writing down the first quantized expression (324), we assumed that the operators acts specifically on states with N particles. On the other hand, (325) acts on the Fock space, i.e. on states where the particle number can take any value. The action of (325) on N-particle states (where N is fixed but arbitrary) is equal to the action of (324).

Derivation of (325)

Let us concentrate on the fermionic case. The bosonic case can be dealt with analogously. We start with our original representation of N-particle states (262)

$$|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle = \mathcal{N} \sum_{P\in S_N} (-1)^{|P|} |\mathbf{r}_1\rangle \otimes \ldots |\mathbf{r}_N\rangle\ . \tag{326}$$

Then

$$\hat{V}|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \sum_{i<j} V(\mathbf{r}_i,\mathbf{r}_j)|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \frac{1}{2}\sum_{i\neq j} V(\mathbf{r}_i,\mathbf{r}_j)|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle \ . \tag{327}$$

On the other hand we know that

$$|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \prod_{j=1}^{N} c^\dagger(\mathbf{r}_j)|0\rangle. \tag{328}$$

Now consider

$$c(\mathbf{r})|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = c(\mathbf{r})\prod_{j=1}^{N} c^\dagger(\mathbf{r}_j)|0\rangle = [c(\mathbf{r}),\prod_{j=1}^{N} c^\dagger(\mathbf{r}_j)\}|0\rangle \ , \tag{329}$$

where is the last step we have used that $c(\mathbf{r})|0\rangle = 0$, and $[A,B\}$ is an anticommutator if both A and B involve an odd number of fermions and a commutator otherwise.
In our case we have a commutator for even N and an anticommutator for odd N.
By repeatedly adding and subtracting terms we find that

$$\begin{aligned}[c(\mathbf{r}),\prod_{j=1}^{N} c^\dagger(\mathbf{r}_j)\} \quad &= \quad \{c(\mathbf{r}),c^\dagger(\mathbf{r}_1)\}\prod_{j=2}^{N} c^\dagger(\mathbf{r}_j) - c^\dagger(\mathbf{r}_1)\{c(\mathbf{r}),c^\dagger(\mathbf{r}_2)\}\prod_{j=3}^{N} c^\dagger(\mathbf{r}_j) \\ &\quad + \ldots + \prod_{j=1}^{N-1} c^\dagger(\mathbf{r}_j)\{c(\mathbf{r}),c^\dagger(\mathbf{r}_N)\}.\end{aligned} \tag{330}$$

Using that $\{c(\mathbf{r}),c^\dagger(\mathbf{r}_j)\} = \delta^{(3)}(\mathbf{r}-\mathbf{r}_j)$ we then find

$$c(\mathbf{r})|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \sum_{n=1}^{N}(-1)^{n-1}\delta^{(3)}(\mathbf{r}-\mathbf{r}_n)\prod_{j\neq n}^{N} c^\dagger(\mathbf{r}_j)|0\rangle = \sum_{n=1}^{N}(-1)^{n-1}\delta^{(3)}(\mathbf{r}-\mathbf{r}_n)|\mathbf{r}_1\ldots\overbrace{\mathbf{r}_n}^{\text{missing}}\ldots\mathbf{r}_N\rangle. \tag{331}$$

Hence

$$\underbrace{c^\dagger(\mathbf{r}')c(\mathbf{r}')}_{\text{number op.}}c(\mathbf{r})|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \sum_{n=1}^{N}(-1)^{n-1}\delta^{(3)}(\mathbf{r}-\mathbf{r}_n)\sum_{m\neq n}^{N}\delta^{(3)}(\mathbf{r}'-\mathbf{r}_m)\ |\mathbf{r}_1\ldots\overbrace{\mathbf{r}_n}^{\text{missing}}\ldots\mathbf{r}_N\rangle, \tag{332}$$

and finally

$$c^\dagger(\mathbf{r})c^\dagger(\mathbf{r}')c(\mathbf{r}')c(\mathbf{r})|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \sum_{n=1}^{N}\delta^{(3)}(\mathbf{r}-\mathbf{r}_n)\sum_{m\neq n}^{N}\delta^{(3)}(\mathbf{r}'-\mathbf{r}_m)\ |\mathbf{r}_1\ldots\mathbf{r}_n\ldots\mathbf{r}_N\rangle. \tag{333}$$

This implies that

$$\frac{1}{2}\int d^3\mathbf{r}d^3\mathbf{r}'\ V(\mathbf{r},\mathbf{r}')\ c^\dagger(\mathbf{r})c^\dagger(\mathbf{r}')c(\mathbf{r}')c(\mathbf{r})|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \frac{1}{2}\sum_{n\neq m} V(\mathbf{r}_n,\mathbf{r}_m)|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle. \tag{334}$$

As $\{|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle\}$ form a basis, this establishes (325).

Derivation of (325)

Using our formula for basis transformations (290)

$$c^\dagger(\mathbf{r}) = \sum_l \langle l|\mathbf{r}\rangle\ c_l^\dagger, \tag{335}$$

we can transform (325) into a general basis. We have

$$\hat{V} \quad = \quad \frac{1}{2}\sum_{ll'mm'}\int d^3\mathbf{r}d^3\mathbf{r}'\ V(\mathbf{r},\mathbf{r}')\langle l|\mathbf{r}\rangle\langle l'|\mathbf{r}'\rangle\langle\mathbf{r}'|m'\rangle\langle\mathbf{r}|m\rangle c_l^\dagger c_{l'}^\dagger c_{m'}c_m \ . \tag{336}$$

We can rewrite this by using that the action of $\hat{V}$ on two-particle states is obtained by taking $N = 2$ in (324), which tells us that $\hat{V}|\mathbf{r}\rangle \otimes |\mathbf{r}'\rangle = V(\mathbf{r}, \mathbf{r}')|\mathbf{r}\rangle \otimes |\mathbf{r}'\rangle$. This implies

$$\begin{aligned} V(\mathbf{r}, \mathbf{r}')\langle l|\mathbf{r}\rangle\langle l'|\mathbf{r}'\rangle\langle \mathbf{r}'|m'\rangle\langle \mathbf{r}|m\rangle &= V(\mathbf{r}, \mathbf{r}') \left[\langle l| \otimes \langle l'|\right] \left[|\mathbf{r}\rangle \otimes |\mathbf{r}'\rangle|\right] \left[\langle \mathbf{r}| \otimes \langle \mathbf{r}'|\right] \left[|m\rangle \otimes |m'\rangle|\right] \\ &= \left[\langle l| \otimes \langle l'|\right] \hat{V} \left[|\mathbf{r}\rangle \otimes |\mathbf{r}'\rangle|\right] \left[\langle \mathbf{r}| \otimes \langle \mathbf{r}'|\right] \left[|m\rangle \otimes |m'\rangle|\right] \end{aligned} \tag{337}$$

Now we use that

$$\int d^3\mathbf{r} d^3\mathbf{r}' \left[|\mathbf{r}\rangle \otimes |\mathbf{r}'\rangle\right] \left[\langle \mathbf{r}| \otimes \langle \mathbf{r}'|\right] = \mathbf{1} \tag{338}$$

to obtain

$$\hat{V} = \frac{1}{2} \sum_{l,l',m,m'} \left[\langle l| \otimes \langle l'|\right] |\hat{V}| \left[|m\rangle \otimes |m'\rangle\right] c_l^\dagger c_{l'}^\dagger c_{m'} c_m. \tag{339}$$

Finally we can express everything in terms of states with the correct exchange symmetry

$$|mm'\rangle = \frac{1}{\sqrt{2}} \left[|m\rangle \otimes |m'\rangle \pm |m'\rangle \otimes |m\rangle\right] \qquad (m \neq m'). \tag{340}$$

in the form

$$\boxed{\hat{V} = \sum_{(ll'),(mm')} \langle ll'|\hat{V}|mm'\rangle c_l^\dagger c_{l'}^\dagger c_{m'} c_m \ .} \tag{341}$$

Here the sums are over a basis of 2-particle states. In order to see that (339) is equal to (341) observe that

$$\sum_{m,m'} [|m\rangle \otimes |m'\rangle] c_{m'} c_m = \frac{1}{2} \sum_{m,m'} [|m\rangle \otimes |m'\rangle \pm |m'\rangle \otimes |m\rangle] c_{m'} c_m = \frac{1}{\sqrt{2}} \sum_{m,m'} |mm'\rangle \ c_{m'} c_m \tag{342}$$

Here the first equality follows from relabelling summation indices $m \leftrightarrow m'$ and using the (anti)commutation relations between c_m and $c_{m'}$ to bring them back in the right order. The second equality follows from the definition of 2-particle states $|mm'\rangle$. Finally we note that because $|mm'\rangle = \pm|m'm\rangle$ (the minus sign is for fermions) we have

$$\frac{1}{\sqrt{2}} \sum_{m,m'} |mm'\rangle \ c_{m'} c_m = \sqrt{2} \sum_{(mm')} |mm'\rangle \ c_{m'} c_m, \tag{343}$$

where the sum is now over a basis of 2-particle states with the appropriate exchange symmetry. The representation (341) generalizes to arbitrary two-particle operators $\mathcal{O}$.

6.5 Homework Question 14

Question 14. Consider the N-particle interaction potential

$$\hat{V} = \sum_{i<j}^{N} V(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j),$$

where $V(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j) = V(\hat{\mathbf{r}}_j, \hat{\mathbf{r}}_i)$. Show that in second quantization it is expressed as

$$\hat{V} = \frac{1}{2} \int d^3\mathbf{r} d^3\mathbf{r}' \ V(\mathbf{r}, \mathbf{r}') \ c^\dagger(\mathbf{r}) c^\dagger(\mathbf{r}') c(\mathbf{r}') c(\mathbf{r}).$$

To do so consider the action of $\hat{V}$ on a basis of N-particle position eigenstates

$$|\mathbf{r}_1 \dots \mathbf{r}_N\rangle = \frac{1}{\sqrt{N! n_1! n_2! \dots}} \sum_P (\pm 1)^{|P|} |\mathbf{r}_1\rangle \otimes |\mathbf{r}_2\rangle \otimes |\mathbf{r}_N\rangle = \frac{1}{\sqrt{n_1! n_2! \dots}} \prod_{j=1}^{N} c^\dagger(\mathbf{r}_j)|0\rangle \ ,$$

where n_j is the occupation number of the j^{th} single-particle state. Argue that in an arbitrary basis of single-particle eigenstates $|l\rangle$ $\hat{V}$ can be expressed in the form

$$\hat{V} = \sum_{ll'mm'} \langle ll'|\hat{V}|mm'\rangle c_l^\dagger c_{l'}^\dagger c_{m'} c_m.$$

7 Application I: The Ideal Fermi Gas

Consider an ideal gas of spin-1/2 fermions. The creation operators in the momentum representation (in the infinite volume) are

$$c_\sigma^\dagger(\mathbf{p}) \ , \quad \sigma = \uparrow, \downarrow . \tag{344}$$

They fulfil canonical anticommutation relations

$$\{c_\sigma(\mathbf{p}), c_\tau(\mathbf{k})\} = 0 = \{c_\sigma^\dagger(\mathbf{p}), c_\tau^\dagger(\mathbf{k})\} \ , \qquad \{c_\sigma(\mathbf{p}), c_\tau^\dagger(\mathbf{k})\} = \delta_{\sigma,\tau}(2\pi\hbar)^3\delta^{(3)}(\mathbf{k}-\mathbf{p}). \tag{345}$$

The Hamiltonian, in the grand canonical ensemble, is

$$H - \mu\hat{N} = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} \underbrace{\left[\frac{\mathbf{p}^2}{2m} - \mu\right]}_{\epsilon(\mathbf{p})} \sum_{\sigma=\uparrow,\downarrow} c_\sigma^\dagger(\mathbf{p}) c_\sigma(\mathbf{p}). \tag{346}$$

Here $\mu > 0$ is the chemical potential. As $c_\sigma^\dagger(\mathbf{p})c_\sigma(\mathbf{p}) = \hat{n}_\sigma(\mathbf{p})$ is the number operator for spin-σ fermions with momentum $\mathbf{p}$, we can easily deduce the action of the Hamiltonian on states in the Fock space:

$$\begin{aligned}
\left[H - \mu\hat{N}\right]|0\rangle &= 0 \ , \\
\left[H - \mu\hat{N}\right] c_\sigma^\dagger(\mathbf{p})|0\rangle &= \epsilon(\mathbf{p})\ c_\sigma^\dagger(\mathbf{p})|0\rangle \ , \\
\left[H - \mu\hat{N}\right] \prod_{j=1}^n c_{\sigma_j}^\dagger(\mathbf{p}_j)|0\rangle &= \left[\sum_{k=1}^n \epsilon(\mathbf{p}_k)\right] \prod_{j=1}^n c_{\sigma_j}^\dagger(\mathbf{p}_j)|0\rangle \ .
\end{aligned} \tag{347}$$

7.1 Quantization in a large, finite volume

In order to construct the ground state and low-lying excitations, it is convenient to work with a discrete set of momenta. This is achieved by considering the gas in a large, periodic box of linear size L. Momentum eigenstates are obtained by solving the eigenvalue equation e.g. in the position representation

$$\hat{\mathbf{p}}\psi_{\mathbf{k}}(\mathbf{r}) = -i\hbar\nabla\psi_{\mathbf{k}}(\mathbf{r}) = \mathbf{k}\psi_{\mathbf{k}}(\mathbf{r}). \tag{348}$$

The solutions are plane waves

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{r}}. \tag{349}$$

Imposing periodic boundary conditions ($\mathbf{e}_a$ is the unit vector in a direction)

$$\psi_{\mathbf{k}}(\mathbf{r} + L\mathbf{e}_a) = \psi_{\mathbf{k}}(\mathbf{r}) \quad \text{for } a = x, y, z, \tag{350}$$

gives quantization conditions for the momenta $\mathbf{k}$

$$e^{\frac{i}{\hbar}Lk_a} = 1 \Rightarrow k_a = \frac{2\pi\hbar n_a}{L} \ , \quad a = x, y, z. \tag{351}$$

To summarize, in a large, periodic box the momenta are quantized as

$$\mathbf{k} = \frac{2\pi\hbar}{L}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} \tag{352}$$

Importantly, we can now normalize the eigenstates to 1, i.e.

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{L^{\frac{3}{2}}} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{r}}. \tag{353}$$

Hence

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \int d^3\mathbf{r}\psi^*_{\mathbf{k}}(\mathbf{r})\psi_{\mathbf{k}'}(\mathbf{r}) = \delta_{\mathbf{k},\mathbf{k}'}. \tag{354}$$

As a consequence of the different normalization of single-particle states, the anticommutation relations of creation/annihilation operators are changed and now read

$$\{c_\sigma(\mathbf{p}), c_\tau(\mathbf{k})\} = 0 = \{c^\dagger_\sigma(\mathbf{p}), c^\dagger_\tau(\mathbf{k})\}\ , \qquad \{c^\dagger_\sigma(\mathbf{p}), c_\tau(\mathbf{k})\} = \delta_{\sigma,\tau}\delta_{\mathbf{k},\mathbf{p}}. \tag{355}$$

The Hamiltonian is

$$\boxed{H - \mu\hat{N} = \sum_{\mathbf{p}} \epsilon(\mathbf{p}) \sum_{\sigma=\uparrow,\downarrow} c^\dagger_\sigma(\mathbf{p}) c_\sigma(\mathbf{p}).} \tag{356}$$

We define a *Fermi momentum* by

$$\frac{p_F^2}{2m} = \mu. \tag{357}$$

7.1.1 Ground State

Then the lowest energy state is obtained by *filling all negative energy single-particle states*, i.e.

$$\boxed{|\mathrm{GS}\rangle = \prod_{|\mathbf{p}|<p_F,\sigma} c^\dagger_\sigma(\mathbf{p})|0\rangle.} \tag{358}$$

The ground state energy is

$$E_{\mathrm{GS}} = \sum_\sigma \sum_{|\mathbf{p}|<p_F} \epsilon(\mathbf{p}). \tag{359}$$

This is extensive (proportional to the volume) as expected. You can see the advantage of working in a finite volume: the product in (358) involves only a finite number of factors and the ground state energy is finite. The ground state momentum is

$$P_{\mathrm{GS}} = \sum_\sigma \sum_{|\mathbf{p}|<p_F} \mathbf{p} = 0. \tag{360}$$

The ground state momentum is zero, because is a state with momentum $\mathbf{p}$ contributes to the sum, then so does the state with momentum $-\mathbf{p}$.

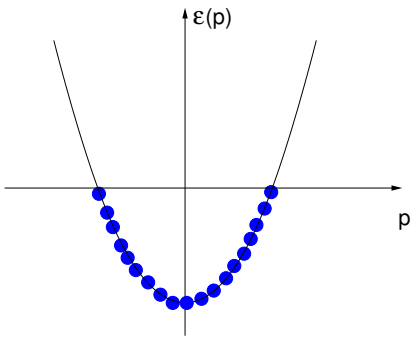


Figure 11: Ground state in the 1 dimensional case. Blue circles correspond to "filled" single-particle states.

7.1.2 Excitations

- Particle excitations

$$c_\sigma^\dagger(\mathbf{k})|\mathrm{GS}\rangle \qquad \text{with } |\mathbf{k}| > p_F. \tag{361}$$

Their energies and momenta are

$$E = E_{\mathrm{GS}} + \epsilon(\mathbf{k}) > E_{\mathrm{GS}}\ , \quad \mathbf{P} = \mathbf{k}. \tag{362}$$

- Hole excitations

$$c_\sigma(\mathbf{k})|\mathrm{GS}\rangle \qquad \text{with } |\mathbf{k}| < p_F. \tag{363}$$

Their energies and momenta are

$$E = E_{\mathrm{GS}} - \epsilon(\mathbf{k}) > E_{\mathrm{GS}}\ , \quad \mathbf{P} = -\mathbf{k}. \tag{364}$$

- Particle-hole excitations

$$c_\sigma^\dagger(\mathbf{k})c_\tau(\mathbf{p})|\mathrm{GS}\rangle \qquad \text{with } |\mathbf{k}| > p_F > |\mathbf{p}|. \tag{365}$$

Their energies and momenta are

$$E = E_{\mathrm{GS}} + \epsilon(\mathbf{k}) - \epsilon(\mathbf{p}) > E_{\mathrm{GS}}\ , \quad \mathbf{P} = \mathbf{k} - \mathbf{p}. \tag{366}$$

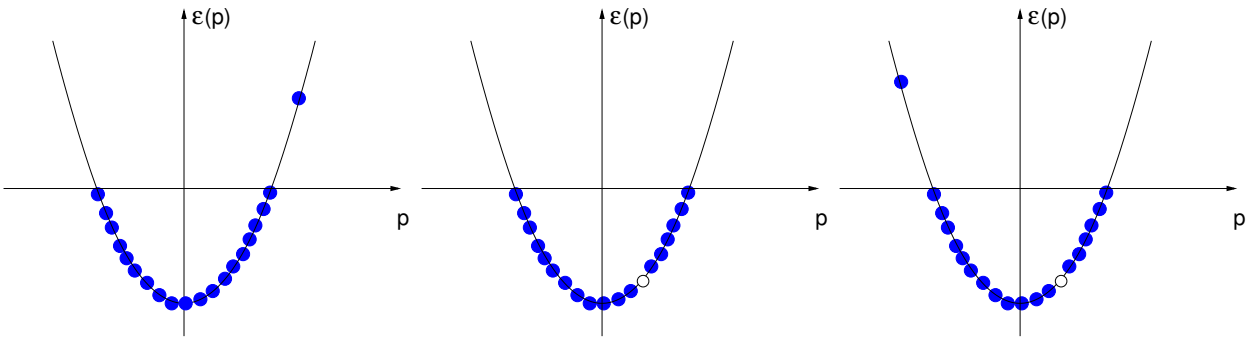


Figure 12: Some simple excited states: (a) particle (b) hole (c) particle-hole.

7.1.3 Density Correlations

Consider the single-particle operator

$$o = |\mathbf{r}\rangle\langle\mathbf{r}| \tag{367}$$

It represents the particle density at position $|\mathbf{r}\rangle$ as can be seen by acting on position eigenstates. In second quantization it is

$$\rho(\mathbf{r}) = \sum_\sigma \int d^3\mathbf{r}' d^3\mathbf{r}''\ \langle\mathbf{r}'|o|\mathbf{r}''\rangle\ c_\sigma^\dagger(\mathbf{r}')c_\sigma(\mathbf{r}'') = \sum_\sigma c_\sigma^\dagger(\mathbf{r})c_\sigma(\mathbf{r}). \tag{368}$$

1. One-point function.

   We now want to determine the expectation value of this operator in the ground state

$$\langle\mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle = \sum_\sigma \langle\mathrm{GS}|c_\sigma^\dagger(\mathbf{r})c_\sigma(\mathbf{r})|\mathrm{GS}\rangle. \tag{369}$$

A crucial observation is that the ground state has a simple description in terms of the Fock space built from momentum eigenstates. Hence what we want to do is to work out the momentum representation of $\rho(\mathbf{r})$. We know from our general formula (291) that

$$c_\sigma(\mathbf{r}) = \sum_{\mathbf{p}} \underbrace{\langle \mathbf{r}|\mathbf{p}\rangle}_{L^{-3/2}e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}} c_\sigma(\mathbf{p}). \tag{370}$$

Substituting this as well as the analogous expression for the creation operator into (369), we obtain

$$\langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle = \sum_\sigma \frac{1}{L^3} \sum_{\mathbf{p},\mathbf{p}'} e^{\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} \langle \mathrm{GS}|c^\dagger_\sigma(\mathbf{p}')c_\sigma(\mathbf{p})|\mathrm{GS}\rangle. \tag{371}$$

For the expectation value $\langle \mathrm{GS}|c^\dagger_\sigma(\mathbf{p}')c_\sigma(\mathbf{p})|\mathrm{GS}\rangle$ to be non-zero, we must have that $c^\dagger_\sigma(\mathbf{p}')c_\sigma(\mathbf{p})|\mathrm{GS}\rangle$ reproduces $|\mathrm{GS}\rangle$ itself. The only way this is possible is if $|\mathbf{p}| < p_F$ (so that the c pokes a hole in the Fermi sea) and $\mathbf{p}' = \mathbf{p}$ (so that the $c^\dagger$ precisely fills the hole made by the c). By this reasoning we have

$$\langle \mathrm{GS}|c^\dagger_\sigma(\mathbf{p}')c_\tau(\mathbf{p})|\mathrm{GS}\rangle = \delta_{\sigma,\tau}\delta_{\mathbf{p},\mathbf{p}'}\theta(p_F - |\mathbf{p}'|). \tag{372}$$

Similarly we can show that

$$\begin{aligned} \langle \mathrm{GS}|c_\sigma(\mathbf{p}')c^\dagger_\tau(\mathbf{p})|\mathrm{GS}\rangle &= \delta_{\sigma,\tau}\delta_{\mathbf{p},\mathbf{p}'}\theta(|\mathbf{p}| - p_F), \\ \langle \mathrm{GS}|c_\sigma(\mathbf{p}')c_\tau(\mathbf{p})|\mathrm{GS}\rangle &= 0 = \langle \mathrm{GS}|c^\dagger_\sigma(\mathbf{p}')c^\dagger_\tau(\mathbf{p})|\mathrm{GS}\rangle. \end{aligned} \tag{373}$$

Substituting (372) back into (371) we find

$$\langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle = \sum_\sigma \frac{1}{L^3} \sum_{\mathbf{p},\mathbf{p}'} e^{\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} \delta_{\mathbf{p},\mathbf{p}'}\ \theta(p_F - |\mathbf{p}|) = \underbrace{2}_{\text{spin}} \frac{1}{L^3} \sum_{\mathbf{p}} \theta(p_F - |\mathbf{p}|) = \frac{N}{L}. \tag{374}$$

So our expectation value gives precisely the particle density. This is expected because our system is translationally invariant and therefore $\langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle$ cannot depend on $\mathbf{r}$.

2. Two-point function.

   Next we want to determine the two-point function

$$\langle \mathrm{GS}|\rho(\mathbf{r})\rho(\mathbf{r}')|\mathrm{GS}\rangle = \sum_{\sigma,\tau} \frac{1}{L^6} \sum_{\mathbf{p},\mathbf{p}'} \sum_{\mathbf{k},\mathbf{k}'} e^{\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} e^{\frac{i}{\hbar}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'} \langle \mathrm{GS}|c^\dagger_\sigma(\mathbf{p}')c_\sigma(\mathbf{p})c^\dagger_\tau(\mathbf{k}')c_\tau(\mathbf{k})|\mathrm{GS}\rangle. \tag{375}$$

   The expectation value $\langle \mathrm{GS}|c^\dagger_\sigma(\mathbf{p}')c_\sigma(\mathbf{p})c^\dagger_\tau(\mathbf{k}')c_\tau(\mathbf{k})|\mathrm{GS}\rangle$ can be calculated by thinking about how the creation and annihilation operators act on the ground state, and then concentrating on the processes that reproduce the ground state itself in the end (see Fig. 13).

The result is

$$\begin{aligned} \langle \mathrm{GS}|c^\dagger_\sigma(\mathbf{p}')c_\sigma(\mathbf{p})c^\dagger_\tau(\mathbf{k}')c_\tau(\mathbf{k})|\mathrm{GS}\rangle &= \delta_{\mathbf{k},\mathbf{k}'}\delta_{\mathbf{p},\mathbf{p}'}\theta(p_F - |\mathbf{p}|)\theta(p_F - |\mathbf{k}|) \\ &\quad + \delta_{\sigma,\tau}\delta_{\mathbf{p},\mathbf{k}'}\delta_{\mathbf{k},\mathbf{p}'}\theta(|\mathbf{k}'| - p_F)\theta(p_F - |\mathbf{k}|). \end{aligned} \tag{376}$$

Observe that by virtue of (372) and (373) this can be rewritten in the form

$$\langle \mathrm{GS}|c^\dagger_\sigma(\mathbf{p}')c_\sigma(\mathbf{p})|\mathrm{GS}\rangle\langle \mathrm{GS}|c^\dagger_\tau(\mathbf{k}')c_\tau(\mathbf{k})|\mathrm{GS}\rangle + \langle \mathrm{GS}|c^\dagger_\sigma(\mathbf{p}')c_\tau(\mathbf{k})|\mathrm{GS}\rangle\langle \mathrm{GS}|c_\sigma(\mathbf{p})c^\dagger_\tau(\mathbf{k}')|\mathrm{GS}\rangle\ . \tag{377}$$

The fact that the 4-point function (376) can be written as a sum over products of two-point functions is a reflection of *Wick's theorem* for noninteracting spin-1/2 fermions. This is not part of the syllabus and we

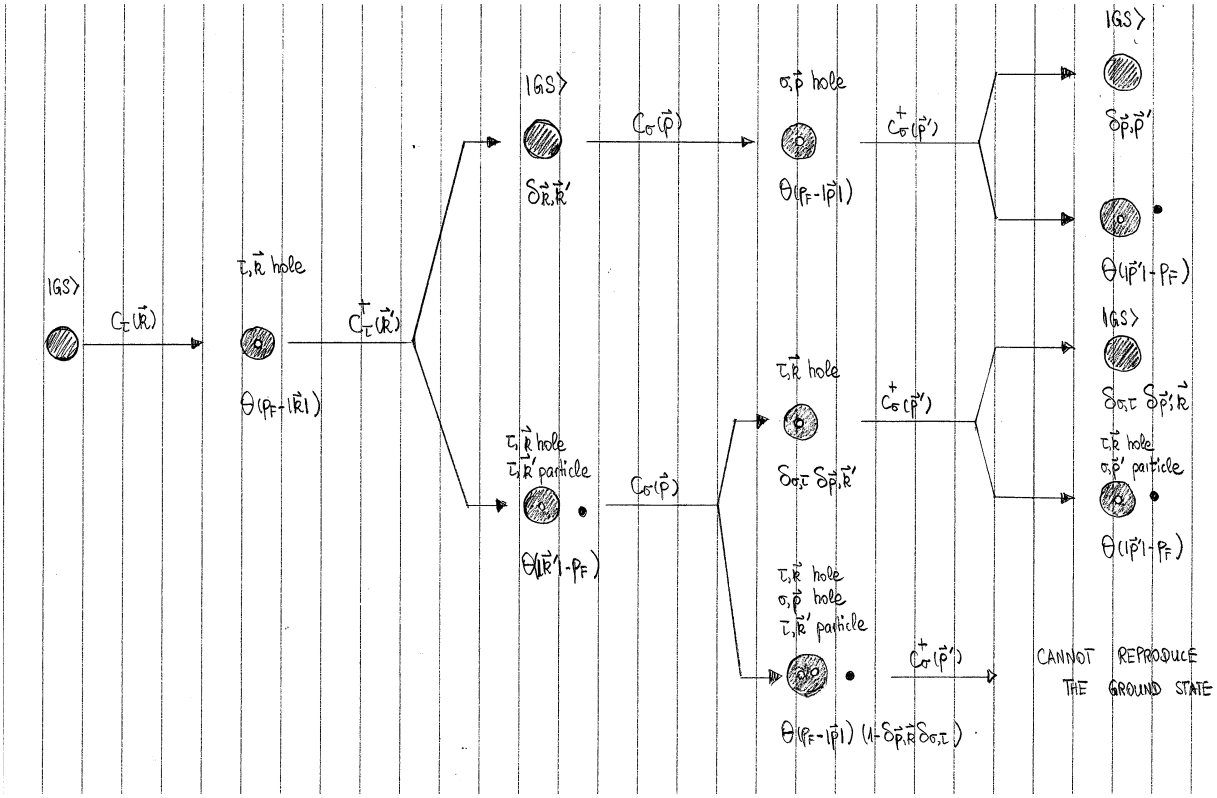


Figure 13:

won't dwell on it, but apart from extra minus signs, this says that $2n$-point functions are given by the sum over all possible "pairings", giving rise to a product of two-point functions. In our particular case this gives

$$\begin{aligned}\langle c^\dagger_\sigma(\mathbf{p}')c_\sigma(\mathbf{p})c^\dagger_\tau(\mathbf{k}')c_\tau(\mathbf{k})\rangle &= \langle c^\dagger_\sigma(\mathbf{p}')c_\sigma(\mathbf{p})\rangle\langle c^\dagger_\tau(\mathbf{k}')c_\tau(\mathbf{k})\rangle - \langle c^\dagger_\sigma(\mathbf{p}')c^\dagger_\tau(\mathbf{k}')\rangle\langle c_\sigma(\mathbf{p})c_\tau(\mathbf{k})\rangle \\ &+ \langle c^\dagger_\sigma(\mathbf{p}')c_\tau(\mathbf{k})\rangle\langle c_\sigma(\mathbf{p})c^\dagger_\tau(\mathbf{k}')\rangle, \end{aligned} \tag{378}$$

and using that the two point function of two creation or two annihilation operators is zero we obtain (377). Substituting (376) back in to (375) gives

$$\begin{aligned}\langle \mathrm{GS}|\rho(\mathbf{r})\rho(\mathbf{r}')|\mathrm{GS}\rangle &= \sum_{\sigma,\sigma'}\frac{1}{L^6}\sum_{\mathbf{k},\mathbf{p}}\theta(p_F-|\mathbf{k}|)\theta(p_F-|\mathbf{p}|) \\ &+ \sum_{\sigma}\frac{1}{L^6}\sum_{\mathbf{k},\mathbf{k}'}\theta(|\mathbf{k}|-p_F)\theta(p_F-|\mathbf{k}'|)e^{\frac{i}{\hbar}(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}-\mathbf{r}')} \\ &= \langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle\langle \mathrm{GS}|\rho(\mathbf{r}')|\mathrm{GS}\rangle + 2\frac{1}{L^3}\sum_{|\mathbf{k}|>p_F}e^{\frac{i}{\hbar}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\frac{1}{L^3}\sum_{|\mathbf{k}'|<p_F}e^{-\frac{i}{\hbar}\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}. \end{aligned} \tag{379}$$

Remark

Evaluting the $\mathbf{k}$ sums for large L: The idea is to turn sums into integrals

$$\begin{aligned}\frac{1}{L^3}\sum_{|\mathbf{k}|<p_F}e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} &\longrightarrow \int\frac{d^3\mathbf{k}}{(2\pi\hbar)^3}\theta(p_F-|\mathbf{k}|)e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} = \int_0^\infty dp p^2\int_0^\pi d\vartheta\sin\vartheta\int_0^{2\pi}d\varphi\,\frac{\theta(p_F-\hbar p)}{(2\pi)^3}e^{ip|\mathbf{R}|\cos\vartheta} \\ &= \int_0^{p_F/\hbar}\frac{dp}{(2\pi)^2}\frac{2p\sin(p|\mathbf{R}|)}{|\mathbf{R}|} = \frac{\sin(p_F|\mathbf{R}|)-p_F|\mathbf{R}|\cos(p_F|\mathbf{R}|)}{2\pi^2|\mathbf{R}|^3}\equiv h(|\mathbf{R}|). \end{aligned} \tag{380}$$

Here we have introduced spherical polar coordinates such that the z-axis of our co-ordinate system is along the $\mathbf{R}$ direction, and

$$\begin{aligned} k_x &= \hbar p \sin\vartheta \cos\varphi \,, \\ k_y &= \hbar p \sin\vartheta \sin\varphi \,, \\ k_z &= \hbar p \cos\vartheta . \end{aligned} \tag{381}$$

The other sum works similarly

$$\frac{1}{L^3} \sum_{|\mathbf{k}|>p_F} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} = \frac{1}{L^3} \sum_{\mathbf{k}} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} - \frac{1}{L^3} \sum_{|\mathbf{k}|<p_F} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} . \tag{382}$$

The second part is evaluated above, while the first part is

$$\frac{1}{L^3} \sum_{\mathbf{k}} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} = \delta^{(3)}(\mathbf{R}). \tag{383}$$

The equality can be proved by multiplying both sides by a test-function $f(\mathbf{R})$ and then integrating over $\mathbf{R}$:

$$\int d^3\mathbf{R} \frac{1}{L^3} \sum_{\mathbf{k}} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} f(\mathbf{R}) = \frac{1}{L^3} \sum_{\mathbf{k}} \int d^3\mathbf{R} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} f(\mathbf{R}) = \frac{1}{L^3} \sum_{\mathbf{k}} \tilde{f}_{\mathbf{k}} = f(\mathbf{0}). \tag{384}$$

Here we have used standard definitions for Fourier series, cf Riley/Hobson/Bence 12.7.

REMARK

Using these simplifications for large L we arrive at our final answer

$$\boxed{\langle \mathrm{GS}|\rho(\mathbf{r})\rho(\mathbf{r}')|\mathrm{GS}\rangle = \langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle^2 + \langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle \delta^{(3)}(\mathbf{r}-\mathbf{r}') - 2\left[h(|\mathbf{r}-\mathbf{r}'|)\right]^2 .} \tag{385}$$

The first two terms are the same as for a *classical* ideal gas, while the third contribution is due to the *fermionic statistics* (Pauli exclusion: "fermions don't like to be close to one another").

7.2 Homework Questions 15-16

Question 15. Consider a system of fermions moving freely on a one-dimensional ring of length L, i.e. periodic boundary conditions are applied between $x = 0$ and $x = L$. The fermions are all in the same spin state, so that spin quantum numbers may be omitted. Fermion creation and annihilation operators at the point x are denoted by $\psi^\dagger(x)$ and $\psi(x)$.
a) Write down the complete set of anticommutation relation satisfied by $\psi^\dagger(x_1)$ and $\psi(x_2)$.
b) Write down the wave-functions of single-particle momentum eigenstates (make sure to take the boundary conditions into account!). What are the allowed values of momentum? Using this result, derive an expression for the momentum space creation and annihilation operators $\Psi_p^\dagger$ and Ψ_p in terms of $\psi^\dagger(x)$ and $\psi(x)$ (hint: use the general result for basis transformation obtained in the lecture notes).
c) Starting with your expression for the anticommutator $\{\psi^\dagger(x_1), \psi(x_2)\}$, evaluate $\{\Psi_p^\dagger, \Psi_q\}$.
d) Derive an expression for $\psi(x)$ in terms of Ψ_k.
e) The density operator $\rho(x)$ is defined by $\rho(x) = \psi^\dagger(x)\,\psi(x)$. The number operator is

$$N = \int_0^L dx\, \rho(x) \,.$$

Express $\rho(x)$ in terms of $\Psi_p^\dagger$ and Ψ_q, and show from this that

$$N = \sum_k \Psi_k^\dagger \Psi_k \,.$$

Let $|0\rangle$ be the vacuum state (containing no particles) and define $|\phi\rangle$ by

$$|\phi\rangle = A\prod_k (u_k + v_k \Psi_k^\dagger)|0\rangle,$$

where u_k and v_k are complex numbers depending on the label k, and A is a normalisation constant.

Evaluate (i) $|A|^2$, (ii) $\langle\phi|N|\phi\rangle$, and (iii) $\langle\phi|N^2|\phi\rangle$. Under what conditions is $|\phi\rangle$ an eigenstate of particle number?

Question 16. Consider a system of fermions in which the functions $\varphi_\ell(x)$, $\ell = 1, 2 \ldots N$, form a complete orthonormal basis for single particle wavefunctions.

a) Explain how Slater determinants may be used to construct a complete orthonormal basis for n-particle states with $n = 2, 3 \ldots N$. Calculate the normalisation constant for such a Slater determinant at a general value of n. How many independent n-particle states are there for each n?

b) Let $C_\ell^\dagger$ and C_ℓ be fermion creation and destruction operators which satisfy the usual anticommutation relations. The quantities a_k are defined by

$$a_k = \sum_{\ell=1}^{N} U_{k\ell} C_\ell,$$

where $U_{k\ell}$ are elements of an $N \times N$ matrix, U. Write down an expression for $a_k^\dagger$. Find the condition which must be satisfied by the matrix U in order that the operators $a_k^\dagger$ and a_k also satisfy fermion anticommutation relations.

c) Non-interacting spinless fermions move in one dimension in an infinite square-well potential, with position coordinate $0 \le x \le L$. The normalised single particle energy eigenstates are

$$\varphi_\ell(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{\ell\pi x}{L}\right),$$

and the corresponding fermion creation operator is $C_\ell^\dagger$.

Write down expressions for $C^\dagger(x)$, the fermion creation operator at the point x, and for $\rho(x)$, the particle density operator, in terms of $C_\ell^\dagger$, C_ℓ and $\varphi_\ell(x)$.

d) What is the ground state expectation value $\langle\rho(x)\rangle$ in a system of n fermions?

In the limit $n \to \infty$, $L \to \infty$, taken at fixed average density $\rho_0 = n/L$, show that

$$\langle\rho(x)\rangle = \rho_0 \left[1 - \frac{\sin 2\pi\rho_0 x}{2\pi\rho_0 x}\right].$$

Sketch this function and comment briefly on its behaviour for $x \to 0$ and $x \to \infty$.

8 Application II: Weakly Interacting Bosons

As you know from Statistical Mechanics, the ideal Bose gas displays the very interesting phenomenon of *Bose condensation*. This has been observed in systems of trapped Rb atoms and led to the award of the Nobel prize in 2001 to Ketterle, Cornell and Wiemann. The atoms in these experiments are bosonic, but the atom-atom interactions are not zero. We now want to understand the effects of interactions in the framework of a microscopic theory. The kinetic energy operator is expressed in terms of creation/annihilation operators single-particle momentum eigenstates as

$$\hat{T} = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} c^\dagger(\mathbf{p}) c(\mathbf{p}). \tag{386}$$

Here we have assumed that our system in enclosed in a large, periodic box of linear dimension L. The boson-boson interaction is most easily expressed in position space

$$\hat{V} = \frac{1}{2}\int d^3\mathbf{r}d^3\mathbf{r}'\ c^\dagger(\mathbf{r})c^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')c(\mathbf{r}')c(\mathbf{r}) \tag{387}$$

A good model for the potential $V(\mathbf{r},\mathbf{r}')$ is to take it of the form

$$V(\mathbf{r},\mathbf{r}') = U\delta^{(3)}(\mathbf{r}-\mathbf{r}'), \tag{388}$$

i.e. bosons interact only if they occupy the same point in space. Changing to the momentum space description

$$c(\mathbf{r}) = \frac{1}{L^{3/2}}\sum_{\mathbf{p}} e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}c(\mathbf{p}), \tag{389}$$

we have

$$\hat{V} = \frac{U}{2L^3}\sum_{\mathbf{p_1},\mathbf{p_2},\mathbf{p_3}} c^\dagger(\mathbf{p_1})c^\dagger(\mathbf{p_2})c(\mathbf{p_3})c(\mathbf{p_1}+\mathbf{p_2}-\mathbf{p_3}). \tag{390}$$

8.1 Ideal Bose Gas

For $U = 0$ we are dealing with an ideal Bose gas and we know that the ground state is a *condensate*: all particles occupy the lowest-energy single-particle state, i.e. the zero-momentum state

$$|\mathrm{GS}\rangle_0 = \frac{1}{\sqrt{N!}}\Big(c^\dagger(\mathbf{p}=\mathbf{0})\Big)^N|0\rangle. \tag{391}$$

So $\mathbf{p} = 0$ is special, and in particular we have

$${}_0\langle\mathrm{GS}|c^\dagger(\mathbf{p}=\mathbf{0})c(\mathbf{p}=\mathbf{0})|\mathrm{GS}\rangle_0 = N. \tag{392}$$

8.2 Bogoliubov Approximation

For small $U > 0$ we expect the Bose-Einstein condensate to persist, i.e. we expect

$$\langle\mathrm{GS}|c^\dagger(\mathbf{p}=\mathbf{0})c(\mathbf{p}=\mathbf{0})|\mathrm{GS}\rangle = N_0 \gg 1. \tag{393}$$

However,

$$[c^\dagger(\mathbf{0})c(\mathbf{0}),\hat{V}] \neq 0, \tag{394}$$

so that the number of $\mathbf{p} = \mathbf{0}$ bosons is not conserved, and the ground state $|\mathrm{GS}\rangle$ will be a superposition of states with different numbers of $\mathbf{p} = \mathbf{0}$ bosons. However, for the ground state and low-lying excited states we will have

$$\langle\Psi|c^\dagger(\mathbf{0})c(\mathbf{0})|\Psi\rangle \simeq N_0\ , \tag{395}$$

where N_0, crucially, is a very large number. The *Bogoliubov approximation* states that, *when acting on the ground state or low-lying excited states*, we in fact have

$$\boxed{c^\dagger(\mathbf{0}) \simeq \sqrt{N_0}\ , \qquad c(\mathbf{0}) \simeq \sqrt{N_0}\ ,} \tag{396}$$

i.e. creation and annihilation operators are approximately diagonal. This is a much stronger statement than (395), and at first sight looks rather strange. It amounts to making an ansatz for low-energy states $|\psi\rangle$ that fulfils

$$\langle\psi'|c(\mathbf{0})|\psi\rangle = \sqrt{N_0}\langle\psi'|\psi\rangle + \ldots \tag{397}$$

where the dots denote terms that are small compared to $\sqrt{N_0}$. We'll return to what this implies for the structure of $|\psi\rangle$ a little later. Using (396) we may expand H in inverse powers of N_0

$$\begin{aligned} H &= \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} c^\dagger(\mathbf{p})c(\mathbf{p}) \\ &\quad + \frac{U}{2L^3}N_0^2 + \frac{UN_0}{2L^3}\sum_{\mathbf{k}\neq\mathbf{0}} 2c^\dagger(\mathbf{k})c(\mathbf{k}) + 2c^\dagger(-\mathbf{k})c(-\mathbf{k}) + c^\dagger(\mathbf{k})c^\dagger(-\mathbf{k}) + c(-\mathbf{k})c(\mathbf{k}) \\ &\quad + \dots \end{aligned} \tag{398}$$

Now use that

$$N_0 = c^\dagger(\mathbf{0})c(\mathbf{0}) = N - \sum_{\mathbf{p}\neq\mathbf{0}} c^\dagger(\mathbf{p})c(\mathbf{p}), \tag{399}$$

where N is the (conserved) total number of bosons, and define

$$\rho = \frac{N}{L^3} = \text{density of particles.} \tag{400}$$

Then our Hamiltonian becomes

$$\boxed{H = \frac{U\rho}{2}N + \sum_{\mathbf{p}\neq\mathbf{0}} \underbrace{\left[\frac{\mathbf{p}^2}{2m} + U\rho\right]}_{\epsilon(\mathbf{p})} c^\dagger(\mathbf{p})c(\mathbf{p}) + \frac{U\rho}{2}\left[c^\dagger(\mathbf{p})c^\dagger(-\mathbf{p}) + c(-\mathbf{p})c(\mathbf{p})\right] + \dots} \tag{401}$$

The Bogoliubov approximation has reduced the complicated four-boson interaction to two-boson terms. The price we pay is that we have to deal with the "pairing"-terms quadratic in creation/annihilation operators.

8.3 Bogoliubov Transformation

Consider the creation/annihilation operators defined by

$$\begin{pmatrix} b(\mathbf{p}) \\ b^\dagger(-\mathbf{p}) \end{pmatrix} = \begin{pmatrix} \cosh(\theta_\mathbf{p}) & \sinh(\theta_\mathbf{p}) \\ \sinh(\theta_\mathbf{p}) & \cosh(\theta_\mathbf{p}) \end{pmatrix} \begin{pmatrix} c(\mathbf{p}) \\ c^\dagger(-\mathbf{p}). \end{pmatrix} \tag{402}$$

It is easily checked that for any choice of Bogoliubov angle $\theta_\mathbf{p}$

$$[b(\mathbf{p}), b(\mathbf{q})] = 0 = [b^\dagger(\mathbf{p}), b^\dagger(\mathbf{q})]\ , \qquad [b(\mathbf{p}), b^\dagger(\mathbf{q})] = \delta_{\mathbf{p},\mathbf{q}}. \tag{403}$$

In terms of the Bogoliubov bosons the Hamiltonian becomes

$$\begin{aligned} H &= \text{const} + \frac{1}{2}\sum_{\mathbf{p}\neq\mathbf{0}} \left[\left(\frac{\mathbf{p}^2}{2m} + U\rho\right)\cosh(2\theta_\mathbf{p}) - U\rho\sinh(2\theta_\mathbf{p})\right]\left[b^\dagger(\mathbf{p})b(\mathbf{p}) + b^\dagger(-\mathbf{p})b(-\mathbf{p})\right] \\ &\quad - \left[\left(\frac{\mathbf{p}^2}{2m} + U\rho\right)\sinh(2\theta_\mathbf{p}) - U\rho\cosh(2\theta_\mathbf{p})\right]\left[b^\dagger(\mathbf{p})b^\dagger(-\mathbf{p}) + b(-\mathbf{p})b(\mathbf{p})\right] + \dots \end{aligned} \tag{404}$$

Now we choose

$$\tanh(2\theta_\mathbf{p}) = \frac{U\rho}{\frac{\mathbf{p}^2}{2m} + U\rho}, \tag{405}$$

as this removes the $b^\dagger b^\dagger + bb$ terms, and leaves us with a *diagonal* Hamiltonian

$$\boxed{H = \text{const} + \sum_{\mathbf{p}\neq\mathbf{0}} E(\mathbf{p})b^\dagger(\mathbf{p})b(\mathbf{p}) + \dots} \tag{406}$$

where

$$E(\mathbf{p}) = \sqrt{\left(\frac{\mathbf{p}^2}{2m} + U\rho\right)^2 - (U\rho)^2} \ . \tag{407}$$

We note that

$$E(\mathbf{p}) \longrightarrow \frac{\mathbf{p}^2}{2m} \qquad \text{for } |\mathbf{p}| \to \infty, \tag{408}$$

which tells us that at high momenta (and hence high energies) we recover the quadratic dispersion. In this limit $\theta_{\mathbf{p}} \to 0$, so that the Bogoliubov bosons reduce to the "physical" bosons we started with. On the other hand

$$E(\mathbf{p}) \longrightarrow \sqrt{\frac{U\rho}{m}}|\mathbf{p}| \qquad \text{for } |\mathbf{p}| \to 0. \tag{409}$$

So here we have a *linear* dispersion.

8.4 Ground State and Low-lying Excitations

We note that the Hamiltonian (406) involves only creation/annihilation operators with $\mathbf{p} \neq 0$. Formally, we can define zero-momentum Bogoliubov bosons as simply being equal to the original ones

$$b(\mathbf{0}) = c(\mathbf{0}) \ . \tag{410}$$

Let us now define the Bogoliubov vacuum state $|\tilde{0}\rangle$ by

$$b(\mathbf{p})|\tilde{0}\rangle = 0 \ . \tag{411}$$

Clearly, for $\mathbf{p} \neq 0$ we have $E(\mathbf{p}) > 0$, and hence no Bogoliubov quasiparticles will be present in the ground state. On the other hand, a basic assumption we made was that

$$\langle \mathrm{GS}|b(\mathbf{0})|\mathrm{GS}\rangle \simeq \sqrt{N_0}. \tag{412}$$

In order to get an idea what this implies for the structure of the ground state, let us express it in the general form

$$|\mathrm{GS}\rangle = \sum_{n=0}^{\infty} \alpha_n \big(b^\dagger(\mathbf{0})\big)^n |\tilde{0}\rangle \ . \tag{413}$$

Eqn (412) then implies that

$$\alpha_{n+1} \simeq \frac{\sqrt{N_0}}{n+1}\alpha_n \ . \tag{414}$$

Replacing this approximate relation by an equality leads to a *coherent state*

$$|\mathrm{GS}\rangle = e^{-N_0/2} e^{\sqrt{N_0} b^\dagger(\mathbf{0})}|\tilde{0}\rangle. \tag{415}$$

Low-lying excited states can now be obtained by creating Bogoliubov quasipartices, e.g.

$$b^\dagger(\mathbf{q})|\mathrm{GS}\rangle, \tag{416}$$

is a particle-excitation with energy $E(\mathbf{q}) > 0$.

8.5 Ground state correlation functions

We are now in a position to work out correlation functions in the ground state such as

$$\langle \mathrm{GS}|c^\dagger(\mathbf{p})c(\mathbf{q})|\mathrm{GS}\rangle \ , \quad \mathbf{p},\mathbf{q}\neq \mathbf{0}. \tag{417}$$

Inverting the Bogoliubov transformation (402) we have

$$\begin{aligned} c^\dagger(\mathbf{p}) &= \cosh(\theta_{\mathbf{p}})b^\dagger(\mathbf{p}) - \sinh(\theta_{\mathbf{p}})b(-\mathbf{p}) \ , \\ c(\mathbf{q}) &= \cosh(\theta_{\mathbf{q}})b(\mathbf{q}) - \sinh(\theta_{\mathbf{q}})b^\dagger(-\mathbf{q}) \ . \end{aligned} \tag{418}$$

Using that

$$\langle \mathrm{GS}|b^\dagger(\mathbf{p}) = 0 = b(\mathbf{q})|\mathrm{GS}\rangle, \tag{419}$$

we find that

$$\begin{aligned} \langle \mathrm{GS}|c^\dagger(\mathbf{p})c(\mathbf{q})|\mathrm{GS}\rangle &= \sinh(\theta_{\mathbf{q}})\sinh(\theta_{\mathbf{q}})\langle \mathrm{GS}|b(-\mathbf{p})b^\dagger(-\mathbf{q})|\mathrm{GS}\rangle \\ &= \sinh^2(\theta_{\mathbf{p}})\delta_{\mathbf{q},\mathbf{p}} \quad (\mathbf{p},\mathbf{q}\neq\mathbf{0}). \end{aligned} \tag{420}$$

This tells us that, in contrast to the ideal Bose gas, in the ground state of the interacting Bose gas we have a finite density of bosons with non-zero momentum

$$\langle \mathrm{GS}|c^\dagger(\mathbf{p})c(\mathbf{p})|\mathrm{GS}\rangle = \sinh^2(\theta_{\mathbf{p}}) \ . \tag{421}$$

Another feature of the ground state is that the two-point function of two annihilation/creation operators is non-zero

$$\langle \mathrm{GS}|c(\mathbf{p})c(\mathbf{q})|\mathrm{GS}\rangle = \langle \mathrm{GS}|c^\dagger(\mathbf{q})c^\dagger(\mathbf{p})|\mathrm{GS}\rangle = -\cosh(\theta_{\mathbf{p}})\sinh(\theta_{\mathbf{q}})\delta_{\mathbf{p},-\mathbf{q}}. \tag{422}$$

These imply that boson number is not a good quantum number in the ground state. More formally, we say that *the ground state spontaneously breaks the U(1) symmetry of the Hamiltonian* $H = \hat{T} + \hat{V}$. Let us explain that statement. The Hamiltonian is invariant under the symmetry operation

$$\begin{aligned} \hat{U}c(\mathbf{p})\hat{U}^\dagger &= e^{i\phi}c(\mathbf{p}) \ , \quad \phi\in\mathbb{R} \ , \\ \hat{U}c^\dagger(\mathbf{p})\hat{U}^\dagger &= e^{-i\phi}c^\dagger(\mathbf{p}) \ , \end{aligned} \tag{423}$$

i.e.

$$\hat{U}H\hat{U}^\dagger = H. \tag{424}$$

The reason for this is that all terms in H involve the same number of creation as annihilation operators, and the total particle number is therefore conserved. This is referred to as a global U(1) symmetry (as the transformations (423) form a group called U(1)). Let us now investigate how ground state expectation values transform. We have

$$\langle \mathrm{GS}|c(\mathbf{p})c(\mathbf{q})|\mathrm{GS}\rangle = \langle \mathrm{GS}|\hat{U}^\dagger\hat{U}c(\mathbf{p})\hat{U}^\dagger\hat{U}c(\mathbf{q})\hat{U}^\dagger\hat{U}|\mathrm{GS}\rangle = e^{2i\phi}\langle \mathrm{GS}|\hat{U}^\dagger c(\mathbf{p})c(\mathbf{q})\hat{U}|\mathrm{GS}\rangle \ . \tag{425}$$

If the ground state were invariant under the symmetry, we would have $\hat{U}|\mathrm{GS}\rangle = |\mathrm{GS}\rangle$. Eqn (425) would then imply that $\langle \mathrm{GS}|c(\mathbf{p})c(\mathbf{q})|\mathrm{GS}\rangle = 0$. Reversing the argument, we see that a non-zero value of the expectation value (422) implies that the ground state *cannot be* invariant under the U(1) symmetry, and in fact *"breaks it spontaneously"*.

8.6 Depletion of the Condensate

We started out by asserting that for small interactions $U > 0$ we retain a Bose-Einstein condensate, i.e. the consensate fraction N_0/N remains large. We can now check that this assumption is *self-consistent*. We have

$$N_0 = N - \sum_{\mathbf{p}\neq\mathbf{0}} c^\dagger(\mathbf{p})c(\mathbf{p}). \tag{426}$$

Thus in the ground state

$$\frac{N_0}{N} = 1 - \frac{1}{N}\sum_{\mathbf{p}\neq\mathbf{0}} \langle \mathrm{GS}|c^\dagger(\mathbf{p})c(\mathbf{p})|\mathrm{GS}\rangle = 1 - \frac{1}{N}\sum_{\mathbf{p}\neq\mathbf{0}} \sinh^2(\theta_{\mathbf{p}}), \tag{427}$$

where we have used (420). This equals

$$\frac{N_0}{N} \;=\; 1 - \frac{1}{2N}\sum_{\mathbf{p}\neq\mathbf{0}} \left[\frac{1}{\sqrt{1-\tanh^2(2\theta_{\mathbf{p}})}} - 1\right] = 1 - \frac{1}{2N}\sum_{\mathbf{p}\neq\mathbf{0}} \left[\frac{1}{\sqrt{1-\left[\frac{U\rho}{\epsilon(\mathbf{p})}\right]^2}} - 1\right]. \tag{428}$$

We again turn this into an integral and evaluate it in spherical polar coordinates, which gives

$$\frac{N_0}{N} \approx 1 - \frac{2\pi}{\rho}\int_0^\infty \frac{dp}{(2\pi\hbar)^3} p^2 \left[\frac{1}{\sqrt{1-\left[\frac{U\rho}{\epsilon(\mathbf{p})}\right]^2}} - 1\right]. \tag{429}$$

By means of the substitution $p = \sqrt{2mU\rho}z$ we can see that the integral is proportional to $U^{3/2}$ and thus indeed small for small U.

9 Application III: Spinwaves in a Ferromagnet

Consider the following model of a magnetic insulator: at each site $\mathbf{r}$ of a D-dimensional with N sites lattice we have a magnetic moment. In QM such magnetic moments are described by three spin-operators

$$S^\alpha_{\mathbf{r}} \;, \quad \alpha = x, y, z \;, \tag{430}$$

which fulfil the angular momentum commutation relations

$$[S^\alpha_{\mathbf{r}}, S^\beta_{\mathbf{r}'}] = \delta_{\mathbf{r},\mathbf{r}'} i\epsilon_{\alpha\beta\gamma} S^\gamma_{\mathbf{r}}. \tag{431}$$

We will assume that the spin are large in the sense that

$$\mathbf{S}^2_{\mathbf{r}} = \sum_\alpha \left(S^\alpha_{\mathbf{r}}\right)^2 = s(s+1) \gg 1. \tag{432}$$

Let us begin by constructing a basis of quantum mechanical states. At each site we have $2s+1$ eigenstates of $S^z_{\mathbf{r}}$

$$S^z_{\mathbf{r}}|m\rangle_{\mathbf{r}} = m|m\rangle_{\mathbf{r}}, \quad m = s, s-1, \ldots, -s. \tag{433}$$

They can be constructed from $|s\rangle_{\mathbf{r}}$ using spin lowering operators $S^-_{\mathbf{r}} = S^x_{\mathbf{r}} - iS^y_{\mathbf{r}}$

$$|s-n\rangle_{\mathbf{r}} = \frac{1}{\mathcal{N}_n}\left(S^-_{\mathbf{r}}\right)^n |s\rangle_{\mathbf{r}} \;, \quad n = 0, 1, \ldots, 2s, \tag{434}$$

where $\mathcal{N}_n$ are normalization constants. A basis of states is then given by

$$\prod_{\mathbf{r}} |s_{\mathbf{r}}\rangle_{\mathbf{r}} \;, \quad -s \le s_{\mathbf{r}} \le s \text{ spin on site } \mathbf{r}. \tag{435}$$

9.1 Heisenberg model and spin-rotational SU(2) symmetry

An appropriate Hamiltonian for a ferromagnetic insulator was derived by Heisenberg

$$\boxed{H = -J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'}.} \tag{436}$$

Here $\langle \mathbf{r}, \mathbf{r}' \rangle$ denote nearest-neighbour pairs of spins and we will assume that $J > 0$. The model (436) is known as the ferromagnetic *Heisenberg model*. You can check that the Hamiltonian (436) commutes with the three total spin operators

$$[H, S^\alpha] = 0 \ , \quad S^\alpha = \sum_{\mathbf{r}} S^\alpha_{\mathbf{r}}. \tag{437}$$

These imply that the Hamiltonian is invariant under general rotations (in spin space)

$$e^{i\boldsymbol{\alpha}\cdot\mathbf{S}} H e^{-i\boldsymbol{\alpha}\cdot\mathbf{S}} = H. \tag{438}$$

The transformations (438) form a group known as SU(2), and the Heisenberg Hamiltonian (436) is invariant under them.

9.2 Exact ground states

One ground state of H is given by

$$\boxed{|\mathrm{GS}\rangle = \prod_{\mathbf{r}} |s\rangle_{\mathbf{r}}.} \tag{439}$$

Its energy is

$$H|\mathrm{GS}\rangle = -J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} s^2 |\mathrm{GS}\rangle = -J s^2 N_B |\mathrm{GS}\rangle, \tag{440}$$

where N_B is the total number of bonds in our lattice. The total spin lowering operator $S^- = \sum_{\mathbf{r}} S^-_{\mathbf{r}}$ commutes with H by virtue of (437) and hence

$$|\mathrm{GS}, n\rangle = \frac{1}{N_n} \left(S^-\right)^n |\mathrm{GS}\rangle \ , \quad 0 \le n \le 2sN \tag{441}$$

are ground states as well (as they have the same energy). Here N_n is a normalization.

Remark

Proof that $|\mathrm{GS}\rangle$ is a ground state:

$$2\mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'} = (\mathbf{S}_{\mathbf{r}} + \mathbf{S}_{\mathbf{r}'})^2 - \mathbf{S}^2_{\mathbf{r}} - \mathbf{S}^2_{\mathbf{r}'} = \mathbf{J}^2 - 2s(s+1). \tag{442}$$

Here $\mathbf{J}^2$ is the total angular momentum squared. Its eigenvalues follow from the theory of adding angular momenta to be

$$\mathbf{J}^2 |j, m\rangle = j(j+1)|j, m\rangle \ , \quad j = 2s, 2s-1, \ldots, 1, 0. \tag{443}$$

This tells us that the maximal eigenvalue of $\mathbf{J}^2$ is $2s(2s+1)$, and by expanding $|\psi\rangle$ in a basis of eigenstates of $\mathbf{J}^2$ we can easily show that

$$\begin{aligned} \langle \psi | \mathbf{J}^2 | \psi \rangle &= \sum_{j,m,j',m'} \langle \psi | j, m \rangle \langle j, m | \mathbf{J}^2 | j', m' \rangle \langle j', m' | \psi \rangle \\ &= \sum_{j,m} |\langle \psi | j, m \rangle|^2 j(j+1) \le 2s(2s+1) \sum_{j,m} |\langle \psi | j, m \rangle|^2 = 2s(2s+1). \end{aligned} \tag{444}$$

This tells us that

$$\langle\psi|\mathbf{S}_{\mathbf{r}}\cdot\mathbf{S}_{\mathbf{r}'}|\psi\rangle \leq s^2. \tag{445}$$

This provides us with a bound on the eigenvalues of the Hamiltonian, as

$$\langle\psi|H|\psi|\rangle \geq -J\sum_{\langle\mathbf{r},\mathbf{r}'\rangle} s^2 = -Js^2Nz. \tag{446}$$

The state we have constructed saturates this bound, so must be a ground state.

REMARK

Let us now see how the SU(2) symmetry is reflected in expectation values of operators $\mathcal{O}$. At finite temperature we have

$$\langle\mathcal{O}\rangle_\beta = \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}\mathcal{O}\right], \tag{447}$$

where $Z(\beta)=\mathrm{Tr}[e^{-\beta H}]$ is the partition function and $\beta = 1/k_BT$. In the $T\to 0$ limit we have

$$\langle\mathcal{O}\rangle_\infty = \frac{1}{2sN+1}\sum_{n=0}^{2sN}\langle \mathrm{GS},\mathrm{n}|\mathcal{O}|\mathrm{GS},\mathrm{n}\rangle, \tag{448}$$

i.e. we average over all ground states. The thermal average, as well as its $T=0$ limit, are invariant under rotations in spin space. Indeed, under a rotation in spin space we have

$$\langle e^{i\boldsymbol{\alpha}\cdot\mathbf{S}}\mathcal{O}e^{-i\boldsymbol{\alpha}\cdot\mathbf{S}}\rangle_\beta = \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}e^{i\boldsymbol{\alpha}\cdot\mathbf{S}}\mathcal{O}e^{-i\boldsymbol{\alpha}\cdot\mathbf{S}}\right] \tag{449}$$

where $\mathbf{S}=\sum_{\mathbf{r}}\mathbf{S}_{\mathbf{r}}$ are the global spin operators. Using the cyclicity of the trace and the fact that H commutes with the global spin operators, we see that this equals $\langle\mathcal{O}\rangle_\beta$. If we choose as our operator $\mathcal{O}$ any of the global spin operators, and consider a rotation by π around one of the orthogonal axes, we see that the magnetization always vanishes

$$\langle S^\alpha\rangle_\beta = 0\ , \quad \alpha = x,y,z. \tag{450}$$

Physically this is what one would expect for a system that is spin rotationally invariant, i.e. looks the same in any direction in spin space.

9.3 Spontaneous Symmetry Breaking

In a real system, the $2sN+1$-fold ground state degeneracy is usually broken through imperfections. In practice the details of these imperfections are not important, the only thing that matters is that the symmetry gets broken. To keep things simple, one retains the spin-rotationally symmetric Hamiltonian, and says that the ground state breaks the symmetry "spontaneously".

A convenient mathematical description of this effect is as follows. Imagine adding an infinitesimal magnetic field $-\epsilon\sum_{\mathbf{r}}S^z_{\mathbf{r}}$ to the Hamiltonian. This will break the symmetry and hence the degeneracy of the ground states, which now will have energies

$$E_{\mathrm{GS,n}} = -Js^2N_B - \epsilon(sN-n). \tag{451}$$

Now consider the sequence of limits

$$\lim_{\epsilon\to 0}\lim_{N\to\infty}\left[E_{\mathrm{GS,n}}-E_{\mathrm{GS},0}\right] = \begin{cases} 0 & \text{if } \lim_{N\to\infty}\frac{n}{N}=0\ , \\ \infty & \text{else.}\end{cases} \tag{452}$$

This means that if we *define* the thermodynamic limit in the above way, then the only surviving ground states will have magnetization per site s, i.e. contain only a non-extensive number of spin flips. In all of these remaining ground states the spin rotational symmetry has been broken. As we have taken $\epsilon\to 0$ our Hamiltonian is again SU(2) symmetric, but the remaining ground states "spontaneously" break this symmetry.

9.4 Holstein-Primakoff Transformation

We succeeded in finding the ground states of H because of their simple structure. For more general spin Hamiltonians, or even the Hamiltonian (436) with negative value of J, this will no longer work and we need a more general, but approximate way of dealing with such problems. This is provided by *(linear) spinwave theory*.

As shown by Holstein and Primakoff, spin operators can be represented in terms of bosonic creation and annihilation operators as follows:

$$S^z_{\mathbf{r}} = s - a^\dagger_{\mathbf{r}} a_{\mathbf{r}} \ , \quad S^+_{\mathbf{r}} = S^x_{\mathbf{r}} + iS^y_{\mathbf{r}} = \sqrt{2s}\sqrt{1 - \frac{a^\dagger_{\mathbf{r}} a_{\mathbf{r}}}{2s}}\, a_{\mathbf{r}} \ . \tag{453}$$

You can check that the bosonic commutation relations

$$[a_{\mathbf{r}}, a^\dagger_{\mathbf{r}'}] = \delta_{\mathbf{r},\mathbf{r}'} \tag{454}$$

imply that

$$[S^\alpha_{\mathbf{r}}, S^\beta_{\mathbf{r}'}] = \delta_{\mathbf{r},\mathbf{r}'} i\epsilon_{\alpha\beta\gamma} S^\gamma_{\mathbf{r}}. \tag{455}$$

However, there is a caveat: the spaces of QM states are different! At site $\mathbf{r}$ we have

$$\big(S_{\mathbf{r}}\big)^n |s\rangle_{\mathbf{r}} \ , \quad n = 0, \ldots, 2s \tag{456}$$

for spins, but for bosons there are infinitely many states

$$\big(a^\dagger_{\mathbf{r}}\big)^n |0\rangle_{\mathbf{r}} \ , \quad n = 0, \ldots, \infty. \tag{457}$$

To make things match, we must impose a *constraint*, that there are at most 2s bosons per site. Now we take advantage of the fact that we have assumed s to be large: in the ground state there are no bosons present, because

$$\langle \mathrm{GS}| s - a^\dagger_{\mathbf{r}} a_{\mathbf{r}} |\mathrm{GS}\rangle = \langle \mathrm{GS}| S^z_{\mathbf{r}} |\mathrm{GS}\rangle = s = \tag{458}$$

Low-lying excited states will only have a few bosons, so for large enough s we don't have to worry about the constraint. Using the Holstein-Primakoff transformation, we can rewrite H in a $1/s$ *expansion*

$$\boxed{H = -J \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} s^2 - s\left[a^\dagger_{\mathbf{r}} a_{\mathbf{r}} + a^\dagger_{\mathbf{r}'} a_{\mathbf{r}'} - a^\dagger_{\mathbf{r}} a_{\mathbf{r}'} - a^\dagger_{\mathbf{r}'} a_{\mathbf{r}}\right] + \ldots} \tag{459}$$

Here the dots indicate terms proportional to s^0, s^{-1}, etc. Once again using that s is large, we drop these terms (for the time being). We then can diagonalize H by going to momentum space

$$a_{\mathbf{r}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} a(\mathbf{k}) \ , \qquad [a(\mathbf{k}), a^\dagger(\mathbf{p})] = \delta_{\mathbf{k},\mathbf{p}} \ , \tag{460}$$

which gives

$$\boxed{H = -Js^2 Nz + \sum_{\mathbf{q}} \epsilon(\mathbf{q}) a^\dagger(\mathbf{q}) a(\mathbf{q}) + \ldots} \tag{461}$$

For a simple cubic lattice the energy is

$$\epsilon(\mathbf{q}) = 2Js\left[3 - \cos q_x - \cos q_x - \cos q_z\right]. \tag{462}$$

For small wave numbers this is quadratic

$$\epsilon(\mathbf{q}) \approx Js|\mathbf{q}|^2 \qquad \text{for } |\mathbf{q}| \to 0. \tag{463}$$

In the context of spontaneous symmetry breaking these gapless excitations are known as *Goldstone modes*.

Let us now revisit the logic underlying our $1/s$ expansion. For things to be consistent, we require that the terms of order s in (461) provide only a small correction to the leading contribution proportional to s^2. This will be the case as long as we are interested only is states $|\Psi\rangle$ such that

$$\langle\Psi|a^\dagger(\mathbf{q})a(\mathbf{q})|\Psi\rangle \ll s. \tag{464}$$

This condition is certainly fulfilled for the ground state and low-lying excited states.

9.4.1 Heisenberg Antiferromagnet

Another example to which spinwave theory can be fruitfully applied is the model

$$H = J\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\mathbf{S}_\mathbf{r}\cdot\mathbf{S}_{\mathbf{r}'}, \tag{465}$$

where $\langle\mathbf{r},\mathbf{r}'\rangle$ denote nearest-neighbour pairs of spins on a simple cubic lattice and $J>0$. Compared to (436) all we have done is to switch the overall sign of H, but this has important consequences. In particular, it is no longer possible to obtain an exact ground state for the model. Instead, we start by considering our spins to be *classical*. This is justified if we are interested only in states with large spin quantum numbers. We will assume this to be the case and check the self-consistency of our assumption later. In the classical limit we can think of the spins as three-dimensional vectors. The lowest energy configuration is then one, where all neighbouring spins point in opposite directions, i.e. along the three cystal axes the spin configuration looks like ↑↓↑↓↑↓ .... This is known as a *Néel state*. It is convenient to subdivide our lattice into two sublattices: on sublattice A all spins point in the same direction, while on sublattice B all spins point in the opposite direction. Like the ferromagnet, the model (465) has a global spin-rotational symmetry, that will be spontaneously broken in the ground state. By choosing our spin quantization axis appropriately, the classical ground state can then be written in the form

$$\prod_{\mathbf{r}\in A}|s\rangle_\mathbf{r}\prod_{\mathbf{r}'\in B}|-s\rangle_{\mathbf{r}'} \tag{466}$$

The idea is now to map this state to a ferromagnetic one, by inverting the spin quantization axis in the B sublattice. After that we can employ the Holstein-Primakoff transformation to carry out a $1/s$ expansion. As a result of the rotation of spin quatization axis on the B sublattice, the part of the Hamiltonian of order s now contains terms involving two annihilation or two creation operators. Diagonalizing the Hamiltonian then requires a Bogoliubov transformation.

9.5 Homework Questions 17-18

Question 17. A magnetic system consists of two types of Heisenberg spin $\mathbf{S}^A$ and $\mathbf{S}^B$ located respectively on the two inter-penetrating sublattices of an NaCl crystal structure (i.e. a simple cubic structure with alternate A and B in any Cartesian direction). Its Hamiltonian is

$$H = J\sum_{i,j}\mathbf{S}_i^A\cdot\mathbf{S}_j^B$$

where the i,j are nearest neighbours, respectively on the A and B sublattices. J is positive. Show that the classical ground state has all the A spins ferromagnetically aligned in one direction and all the B spins ferromagnetically aligned in the opposite direction. Assume the quantum mechanical ground state is well approximated by the classical one. To a first approximation the spin operators are given in terms of boson operators a,b by

A sublattice	B sublattice
$S_i^z = S^A - a_i^\dagger a_i$	$S_j^z = -S^B + b_j^\dagger b_j$
$S_i^+ \equiv S_i^x + \mathrm{i}S_i^y \simeq (2S^A)^{1/2}a_i$	$S_j^+ \equiv S_j^x + \mathrm{i}S_j^y \simeq (2S^B)^{1/2}b_j^\dagger$
$S_i^- \equiv S_i^x - \mathrm{i}S_i^y \simeq (2S^A)^{1/2}a_i^\dagger$	$S_j^- \equiv S_j^x - \mathrm{i}S_j^y \simeq (2S^B)^{1/2}b_j$

Discuss the validity of this approximation. Use these relations to express the Hamiltonian in terms of the boson operators to quadratic order.

Transforming to crystal momentum space using (with N the number of sites on one sublattice)

$$a_i = N^{-1/2} \sum_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i} a_{\mathbf{k}}, \quad b_j = N^{-1/2} \sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_j} b_{\mathbf{k}}$$

show that your result can be expressed in the form

$$H = E_0 + \sum_{\mathbf{k}} \left[A_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + B_{\mathbf{k}} b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + C_{\mathbf{k}} (a^\dagger_{\mathbf{k}} b^\dagger_{\mathbf{k}} + b_{\mathbf{k}} a_{\mathbf{k}}) \right]$$

and determine the coefficients. Hence calculate the spectrum of excitations at low momenta. Consider both the cases with $S^A = S^B$ and $S^A \neq S^B$ and comment on your results.

Question 18. (optional) Consider the ideal Fermi gas at finite density N/V in a periodic 3-dimensional box of length L.
(a) Give an expression of the ground state in terms of creation operators for momentum eigenstates.
(b) Calculate the **single-particle Green's function**

$$\begin{aligned} G_{\sigma\tau}(\omega, \mathbf{q}) &= \int dt\ e^{i\omega(t-t')} \int d^3\mathbf{r}\ e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} G_{\sigma\tau}(t, \mathbf{r}; t', \mathbf{r}')\ , \\ G_{\sigma\tau}(t, \mathbf{r}; t', \mathbf{r}') &= -i\langle GS | T c_\sigma(\mathbf{r}, t)\ c^\dagger_\tau(\mathbf{r}', t') | GS \rangle, \end{aligned} \tag{467}$$

where T denotes time-ordering (i.e. $T\mathcal{O}(t_1)\mathcal{O}(t_2) = \theta(t_1 - t_2)\mathcal{O}(t_1)\mathcal{O}(t_2) - \theta(t_2 - t_1)\mathcal{O}(t_2)\mathcal{O}(t_1)$ for fermionic operators), and

$$c_\sigma(\mathbf{r}, t) \equiv e^{\frac{i}{\hbar}Ht} c_\sigma(\mathbf{r}) e^{-\frac{i}{\hbar}Ht}. \tag{468}$$

First express the creation/annihilation operators $c^\dagger_\sigma(\mathbf{r}, t)$, $c_\sigma(\mathbf{r}, t)$ in terms of creation/annihilation operators in momentum space $c^\dagger_\sigma(\mathbf{p}, t)$, $c_\sigma(\mathbf{p}, t)$. Then show that for annihilation operators in momentum space we have

$$c_\sigma(\mathbf{p}, t) \equiv e^{\frac{i}{\hbar}Ht} c_\sigma(\mathbf{p}) e^{-\frac{i}{\hbar}Ht} = c_\sigma(\mathbf{p}) e^{-\frac{i}{\hbar}t\epsilon(\mathbf{p})}\ , \tag{469}$$

where $\epsilon(\mathbf{p}) = \mathbf{p}^2/2m - \mu$. Use this to show that

$$c_\sigma(\mathbf{r}, t) = \frac{1}{L^{3/2}} \sum_{\mathbf{p}} e^{-\frac{i}{\hbar}t\epsilon(\mathbf{p}) + i\mathbf{p}\cdot\mathbf{r}}\ c_\sigma(\mathbf{p}). \tag{470}$$

Now insert (470) into (467) and evaluate the ground state expectation value to obtain an integral representation for $G_{\sigma\tau}(t, \mathbf{r}; t', \mathbf{r}')$. Why does the Green's function only depend on $t - t'$ and $\mathbf{r} - \mathbf{r}'$? Finally, calculate $G_{\sigma\tau}(\omega, \mathbf{q})$.

Note: the imaginary part of the single-particle Green's function is (approximately) measured by angle resolved photoemission (ARPES) experiments.

10 Path Integral for interacting Bose systems

A key ingredient in our construction of the path integral for a single particle was the resolution of the identity

$$\mathbf{1} = \int dx\ |x\rangle\langle x|\ , \tag{471}$$

which allowed us to break up $e^{-\beta H}$ into a product over infinitesimal propagators.

10.1 Coherent States

In order to deal with many-boson systems, we require a convenient analog on the Fock space. This is provided by *coherent states*

$$\boxed{|\boldsymbol{\phi}\rangle = \exp\left(\sum_\ell \phi_\ell a_\ell^\dagger\right)|0\rangle\ , \quad \phi_\ell \in \mathbb{C}\ ,} \tag{472}$$

where a_ℓ denotes the bosonic annihilation operator for the single-particle state labeled by ℓ and $|0\rangle$ is the Fock vacuum. If N_{SP} is the number of single-particle states, then $\boldsymbol{\phi}$ is a N_{SP}-dimensional complex vector. The states (472) are simultaneous eigenstates of all annihilation operators

$$\boxed{a_j|\boldsymbol{\phi}\rangle = \phi_j|\boldsymbol{\phi}\rangle.} \tag{473}$$

In order to prove (473) consider

$$a_j|\boldsymbol{\phi}\rangle = a_j \exp\left(\sum_\ell \phi_\ell a_\ell^\dagger\right)|0\rangle = \left[a_j, \exp\left(\sum_\ell \phi_\ell a_\ell^\dagger\right)\right]|0\rangle = \exp\left(\sum_{\ell\neq j} \phi_\ell a_\ell^\dagger\right)\left[a_j, \exp\left(\phi_j a_j^\dagger\right)\right]|0\rangle. \tag{474}$$

The commutator is easily calculated by expanding the exponential in its power series

$$\left[a_j, \exp\left(\phi_j a_j^\dagger\right)\right] = \phi_j \exp\left(\phi_j a_j^\dagger\right), \tag{475}$$

and substituting this back into (474) establishes (473). Coherent states are *not* mutually orthogonal. In fact, they fulfil

$$\boxed{\langle\boldsymbol{\psi}|\boldsymbol{\phi}\rangle = e^{\sum_\ell \psi_\ell^* \phi_\ell}.} \tag{476}$$

This result for the scalar product can be obtained by applying the Baker-Campbell-Hausdorff (BCH) formula, which states that for two operators such that $[A,[A,B]] = 0 = [B,[A,B]]$ we have

$$e^A e^B = e^{A+B} e^{\frac{1}{2}[A,B]} = e^B e^A e^{[A,B]}\ . \tag{477}$$

Setting $A = \sum_\ell \psi_\ell^* a_\ell$, $B = \sum_j \phi_j a_j^\dagger$, using the BCH formula, and then noting that $A|0\rangle = 0 = \langle 0|B$, we obtain (476). While coherent states do not form an orthogonal set, they nevertheless provide a resolution of the identity on the Fock space

$$\boxed{\mathbf{1} = \int \underbrace{\prod_j \frac{d^2\phi_j}{\pi}}_{d(\boldsymbol{\phi},\boldsymbol{\phi}^*)} e^{-\sum_\ell |\phi_\ell|^2}\ |\boldsymbol{\phi}\rangle\langle\boldsymbol{\phi}|.} \tag{478}$$

Here $d^2\phi_\ell$ denotes the integration over the complex variable ϕ_ℓ, e.g. in polar co-ordinates we have

$$\int d^2\phi_j = \int_0^\infty dr_j r_j \int_0^{2\pi} d\varphi_j\ , \quad \phi_j = r_j e^{i\varphi_j}. \tag{479}$$

To prove (478) we note that

$$\begin{aligned} |\boldsymbol{\phi}\rangle &= e^{\phi_1 a_1^\dagger}\ e^{\phi_2 a_2^\dagger}\ e^{\phi_3 a_3^\dagger} \ldots |0\rangle = \sum_{n_1=0}^\infty \frac{(\phi_1)^{n_1}}{n_1!} \sum_{n_2=0}^\infty \frac{(\phi_2)^{n_2}}{n_2!} \ldots (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}(a_3^\dagger)^{n_3} \ldots |0\rangle \\ &= \sum_{n_1=0}^\infty \frac{(\phi_1)^{n_1}}{\sqrt{n_1!}} \sum_{n_2=0}^\infty \frac{(\phi_2)^{n_2}}{\sqrt{n_2!}} \sum_{n_3=0}^\infty \frac{(\phi_3)^{n_3}}{\sqrt{n_3!}} \ldots |n_1 n_2 n_3 \ldots\rangle\ , \end{aligned} \tag{480}$$

where $|n_1 n_2 \dots\rangle$ is a state in the occupation number representation. Hence

$$|\boldsymbol{\phi}\rangle\langle\boldsymbol{\phi}| = \sum_{n_1,n_2,\dots} \sum_{m_1,m_2,\dots} \frac{\phi_1^{n_1}(\phi_1^*)^{m_1}\phi_2^{n_2}(\phi_2^*)^{m_2}\dots}{\sqrt{n_1!m_1!n_2!m_2!\dots}} |n_1 n_2 n_3 \dots\rangle\langle m_1 m_2 m_3 \dots| \ . \tag{481}$$

Inspection of (478) and (481) shows that the integral over ϕ_j and ϕ_j^* is

$$\int_0^\infty dr_j \int_0^{2\pi} d\varphi_j \ r^{n_j+m_j+1} e^{-r_j^2} e^{i\varphi(n_j-m_j)} = n_j! \ \delta_{n_j,m_j} \ . \tag{482}$$

Carrying out all integrals we obtain

$$\int d(\boldsymbol{\phi},\boldsymbol{\phi^*}) e^{-\sum_\ell |\phi_\ell|^2} \ |\boldsymbol{\phi}\rangle\langle\boldsymbol{\phi}| = \sum_{n_1,n_2,\dots} |n_1 n_2 n_3 \dots\rangle\langle n_1 n_2 n_3 \dots| \ . \tag{483}$$

The right hand side is a resolution of the identity in the occupation number representation.

10.2 Partition Function

Let us now consider a general many-boson Hamiltonian of the form

$$\boxed{\hat{H} = \sum_{i,j} h_{ij} a_i^\dagger a_j + \sum_{i,j,k,l} V_{ijkl} a_i^\dagger a_j^\dagger a_k a_l.} \tag{484}$$

We first want to derive a path integral representation for the partition function

$$Z(\beta) = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right] = \sum_n \langle n|e^{-\beta\hat{H}}|n\rangle. \tag{485}$$

Inserting a resolution of the identity in terms of coherent states this can rewritten as

$$\begin{aligned} \int d(\boldsymbol{\psi},\boldsymbol{\psi^*}) e^{-\sum_\ell |\psi_\ell|^2} \sum_n \langle n|\boldsymbol{\psi}\rangle \ \langle\boldsymbol{\psi}|e^{-\beta\hat{H}}|n\rangle &= \int d(\boldsymbol{\psi},\boldsymbol{\psi^*}) e^{-\sum_\ell |\psi_\ell|^2} \sum_n \langle\boldsymbol{\psi}|e^{-\beta\hat{H}}|n\rangle\langle n|\boldsymbol{\psi}\rangle \\ &= \int d(\boldsymbol{\psi},\boldsymbol{\psi^*}) e^{-\sum_\ell |\psi_\ell|^2} \langle\boldsymbol{\psi}|e^{-\beta\hat{H}}|\boldsymbol{\psi}\rangle. \end{aligned} \tag{486}$$

In the next step we break up $e^{-\beta H}$

$$e^{-\beta H} = e^{-\epsilon H} e^{-\epsilon H} \dots e^{-\epsilon H} \ , \quad \epsilon = \frac{\beta}{N}, \tag{487}$$

and then insert resolutions of the identity between each of the factors. This leaves us with matrix elements of the form

$$\begin{aligned} \langle\boldsymbol{\psi}^{(n+1)}|e^{-\epsilon\hat{H}}|\boldsymbol{\psi}^{(n)}\rangle &= \langle\boldsymbol{\psi}^{(n+1)}|\mathbf{1} - \epsilon\hat{H}|\boldsymbol{\psi}^{(n)}\rangle + \mathcal{O}(\epsilon^2) \\ &= \langle\boldsymbol{\psi}^{(n+1)}|\boldsymbol{\psi}^{(n)}\rangle \left[1 - \epsilon H\big(\boldsymbol{\psi}^{(n+1)^*}, \boldsymbol{\psi}^{(n)}\big)\right] + \mathcal{O}(\epsilon^2) \\ &= \langle\boldsymbol{\psi}^{(n+1)}|\boldsymbol{\psi}^{(n)}\rangle \ e^{-\epsilon H\left(\boldsymbol{\psi}^{(n+1)^*}, \boldsymbol{\psi}^{(n)}\right)} + \mathcal{O}(\epsilon^2) \ , \end{aligned} \tag{488}$$

where

$$H\big(\boldsymbol{\psi}^*, \boldsymbol{\psi}'\big) = \sum_{i,j} h_{ij}\psi_i^*\psi_j' + \sum_{i,j,k,l} V_{ijkl}\psi_i^*\psi_j^*\psi_k'\psi_l'. \tag{489}$$

In going from the first to the second line in (488) we have used that

$$a_j|\boldsymbol{\psi'}\rangle = \psi_j'|\boldsymbol{\psi'}\rangle \ , \quad \langle\boldsymbol{\psi}|a_i^\dagger = \psi_i^*\langle\boldsymbol{\psi}| \ . \tag{490}$$

After these steps we end up with a representation of the form

$$Z(\beta) = \lim_{N\to\infty} \int \prod_{m=1}^{N} \int d(\boldsymbol{\psi}^{(m)}, \boldsymbol{\psi}^{(m)^*}) \ \exp\left[-\epsilon \sum_{n=0}^{N-1} \Big(\frac{\boldsymbol{\psi}^{(n)^*} - \boldsymbol{\psi}^{(n+1)^*}}{\epsilon} \Big) \cdot \boldsymbol{\psi}^{(n)} + H\big(\boldsymbol{\psi}^{(n+1)^*}, \boldsymbol{\psi}^{(n)}\big) \right]. \quad (491)$$

In complete analogy to what we did in the single-particle case, we can now interpret the sequence $\boldsymbol{\psi}^{(1)}$, $\boldsymbol{\psi}^{(2)}$,$\ldots$ $\boldsymbol{\psi}^{(N-1)}$ as a discretization of a path on the space of N_{SP} dimensional complex vectors

$$\boldsymbol{\psi}(\tau_n) = \boldsymbol{\psi}^{(n)} \ , \quad \tau_n = n\epsilon. \quad (492)$$

In the limit $N \to \infty$ this goes over into a vector-valued function of imaginary time $\boldsymbol{\psi}(\tau)$, and the partition function acquires the following formal expression

$$Z(\beta) = \int \mathcal{D}\big(\boldsymbol{\psi}^*(\tau), \boldsymbol{\psi}(\tau)\big) \ e^{-S[\boldsymbol{\psi}^*(\tau), \boldsymbol{\psi}(\tau)]} \ , \quad (493)$$

where the action S is given by

$$S[\boldsymbol{\psi}^*(\tau), \boldsymbol{\psi}(\tau)] = \int_0^\beta d\tau \left[\sum_{i,j} h_{ij} \psi_i^*(\tau) \left[\partial_\tau + h_{ij}\right] \psi_j(\tau) + \sum_{i,j,k,l} V_{ijkl} \psi_i^*(\tau) \psi_j^*(\tau) \psi_k(\tau) \psi_l(\tau) \right]. \quad (494)$$