Lecture Notes for the C6 Theory Option

F.H.L. Essler
The Rudolf Peierls Centre for Theoretical Physics
Oxford University, Oxford OX1 3NP, UK

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Please report errors and typos to fab@thphys.ox.ac.uk

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 do so 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).

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

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

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

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]

[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".

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

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. 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

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

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).

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.

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

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

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,

$$\begin{aligned} I(z)^2 &= \int_{-\infty}^{\infty} dy_1\, \exp(-\frac{1}{2}zy_1^2) \int_{-\infty}^{\infty} dy_2\, \exp(-\frac{1}{2}zy_2^2) = \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2\, \exp(-\frac{1}{2}z(y_1^2+y_2^2)) \qquad (24)\\ &= \int_0^{2\pi} d\varphi \int_0^{\infty} dr\, r \exp(-\frac{1}{2}zr^2) = \frac{2\pi}{z}\,. \qquad (25) \end{aligned}$$

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

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

2 Path Integrals in Quantum Mechanics

So far you have encountered two ways of doing QM

1. solving the Schrödinger equation for the wave function ($\rightarrow$ PDEs);
2. following Heisenberg, we can work with operators, commutation relations, eigenstates.

Historically it took some time for people to realize that these are in fact equivalent.

There is a third approach to QM, due to *Feynman*. It is particularly useful for QFTs and many-particle QM problems, as it makes certain calculations much easier. We will now introduce this approach.

2.1 The Propagator

Our starting point is the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle. \tag{35}$$

We recall that the wave function is given by

$$\psi(\vec{x},t) = \langle\vec{x}|\psi(t)\rangle. \tag{36}$$

Eqn (35) can be integrated to give

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi(0)\rangle \tag{37}$$

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

$$U(t;t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}. \tag{38}$$

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

$$\boxed{\langle\vec{x}'|U(t;t_0)|\vec{x}\rangle\ ,} \tag{39}$$

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

$$H = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + V(\hat{x}). \tag{40}$$

We want to calculate the propagator

$$\langle x_N|U(t;0)|x_0\rangle. \tag{41}$$

It is useful to introduce small time steps

$$t_n = n\epsilon \ , \quad n = 0, \ldots, N, \tag{42}$$

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

$$U(t;0) = \left(e^{-\frac{i}{\hbar}H\epsilon}\right)^N . \tag{43}$$

The propagator is

$$\begin{aligned} \langle x_N|U(t;0)|x_0\rangle &= \langle x_N|e^{-\frac{i}{\hbar}H\epsilon}\cdots e^{-\frac{i}{\hbar}H\epsilon}|x_0\rangle \\ &= \int dx_{N-1}\ldots\int dx_1\ \langle x_N|e^{-\frac{i}{\hbar}H\epsilon}|x_{N-1}\rangle\langle x_{N-1}|e^{-\frac{i}{\hbar}H\epsilon}|x_{N-2}\rangle\ldots\langle x_1|e^{-\frac{i}{\hbar}H\epsilon}|x_0\rangle, \end{aligned} \tag{44}$$

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

$$\mathbf{1} = \int dx\ |x\rangle\langle x| \ . \tag{45}$$

This expression now has a very nice and intuitive interpretation, see Fig. 1:

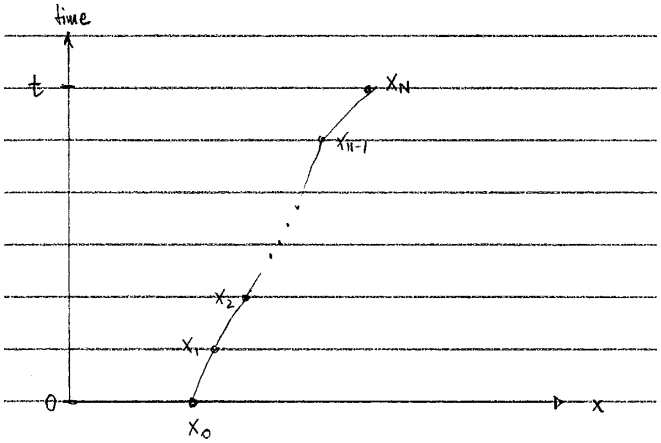


Figure 1: Propagator as sum over paths.

The propagator, i.e. the 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"

$$\langle x_{n+1}|e^{-\frac{i}{\hbar}H\epsilon}|x_n\rangle. \tag{46}$$

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

$$e^{\alpha(\hat{T}+\hat{V})} \neq e^{\alpha\hat{T}}e^{\alpha\hat{V}}. \tag{47}$$

However, using that ϵ is infinitesimal, we have

$$\begin{aligned} e^{-\frac{i}{\hbar}\epsilon(\hat{T}+\hat{V})} &= 1-\frac{i}{\hbar}\epsilon(\hat{T}+\hat{V})+\mathcal{O}(\epsilon^2)\ , \\ e^{-\frac{i}{\hbar}\epsilon\hat{T}}e^{-\frac{i}{\hbar}\epsilon\hat{V}} &= 1-\frac{i}{\hbar}\epsilon(\hat{T}+\hat{V})+\mathcal{O}(\epsilon^2). \end{aligned} \tag{48}$$

So up to terms of order ϵ^2 we have

$$\langle x_{n+1}|e^{-\frac{i}{\hbar}H\epsilon}|x_n\rangle \simeq \langle x_{n+1}|e^{-\frac{i}{\hbar}\hat{T}\epsilon}e^{-\frac{i}{\hbar}\hat{V}\epsilon}|x_n\rangle = \langle x_{n+1}|e^{-\frac{i}{\hbar}\hat{T}\epsilon}|x_n\rangle e^{-\frac{i}{\hbar}V(x_n)\epsilon}, \tag{49}$$

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

$$\begin{aligned} \langle x_{n+1}|e^{-\frac{i}{\hbar}\hat{T}\epsilon}|x_n\rangle &= \int\frac{dp}{2\pi}\langle x_{n+1}|e^{-\frac{ip^2\epsilon}{2m\hbar}}|p\rangle\langle p|x_n\rangle = \int\frac{dp}{2\pi\hbar}e^{-\frac{ip^2\epsilon}{2m\hbar}-i\frac{p}{\hbar}(x_n-x_{n+1})} \\ &= \frac{m}{2\pi i\hbar\epsilon}e^{\frac{im}{2\hbar\epsilon}(x_n-x_{n+1})^2}. \end{aligned} \tag{50}$$

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

$$\langle x|p\rangle = e^{\frac{ipx}{\hbar}}. \tag{51}$$

The integral over p is performed by chaging variables to $p' = p - \frac{m}{\epsilon}(x_n - x_{n+1})$. Substituting (50) and (49) back into our expression (44) for the propagator gives

$$\boxed{\langle x_N|U(t;0)|x_0\rangle = \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}}\int dx_1\ldots dx_{N-1}\exp\left(\frac{i\epsilon}{\hbar}\sum_{n=0}^{N-1}\frac{m}{2}\left(\frac{x_{n+1}-x_n}{\epsilon}\right)^2-V(x_n)\right)} \tag{52}$$

Note that in this expression there are no operators left.

2.1.1 Propagator as a "Functional Integral"

The way to think about (52) 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

$$\frac{x_{n+1}-x_n}{\epsilon} = \frac{x(t_{n+1})-x(t_n)}{t_{n+1}-t_n} \simeq \dot{x}(t_n), \tag{53}$$

and

$$\epsilon\sum_{n=0}^{N-1}\frac{m}{2}\left(\frac{x_{n+1}-x_n}{\epsilon}\right)^2-V(x_n) \simeq \int_0^t dt'\left[\frac{m}{2}\dot{x}^2(t')-V(x)\right] \equiv \int_0^t dt'\mathcal{L}[\dot{x},x], \tag{54}$$

where $\mathcal{L}$ is the *Lagrangian* of the system. In classical mechanics the time-integral of the Lagrangian is known as the *action*

$$S = \int_0^t dt'\mathcal{L}. \tag{55}$$

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

- 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 (52) 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*

$$\boxed{\langle x_N|U(t;0)|x_0\rangle = \mathcal{N}\int \mathcal{D}x(t')\; e^{\frac{i}{\hbar}S[x(t')]}.} \tag{56}$$

What is in fact meant by (56) is the limit of the discretized expression (52). The ultimate utility of (56) 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. The probability amplitude for propagation from x_0 to 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!

2.2 Classical Limit and Stationary Phase Approximation

An important feature of (56) 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

$$g(a) = \int_{-\infty}^{\infty} dt\; h_1(t)e^{iah_2(t)}, \tag{57}$$

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

$$h_2'(t) = 0. \tag{58}$$

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

$$g(a \gg 1) \approx \int_{-\infty}^{\infty} dt\left[h_1(t_0) + (t-t_0)h_1'(t_0) + \ldots\right] e^{iah_2(t_0) + i\frac{ah_2''(t_0)}{2}(t-t_0)^2}, \tag{59}$$

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)

$$g(a \gg 1) \approx \sqrt{\frac{2\pi i}{ah_2''(t_0)}}h_1(t_0)e^{iah_2(t_0)}\ . \tag{60}$$

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

$$\frac{\delta S}{\delta x(t')} = 0. \tag{61}$$

The condition (61) precisely defines the *classical trajectories* $x(t')$!

2.3 The Propagator for Free Particles

We now wish to calculate the functional integral (56) for a free particle, i.e.

$$V(x) = 0. \tag{62}$$

Going back to the explicit expression (52) we have

$$\langle x_N|U(t;0)|x_0\rangle = \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}}\int dx_1\ldots dx_{N-1}\exp\left(\frac{i\epsilon}{\hbar}\sum_{n=0}^{N-1}\frac{m}{2}\left(\frac{x_{n+1}-x_n}{\epsilon}\right)^2\right). \tag{63}$$

It is useful to change integration variables to

$$y_j = x_j - x_N\ , \quad j = 1,\ldots,N-1, \tag{64}$$

which leads to an expression

$$\langle x_N|U(t;0)|x_0\rangle = \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}}\int d\mathbf{y}\exp\left(-\frac{1}{2}\mathbf{y}^T\mathbf{A}\mathbf{y}+\mathbf{J}^T\cdot\mathbf{y}\right)e^{\frac{im}{2\hbar\epsilon}(x_0-x_N)^2}. \tag{65}$$

Here

$$\mathbf{J}^T = \left(\frac{im}{\hbar\epsilon}(x_N-x_0),0,\ldots,0\right), \tag{66}$$

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

$$A_{jk} = \frac{-im}{\epsilon\hbar}\left[2\delta_{j,k}-\delta_{j,k+1}-\delta_{j,k-1}\right]. \tag{67}$$

For a given N (65) is a multidimensional Gaussian integral and can be carried out using (34)

$$\langle x_N|U(t;0)|x_0\rangle = \lim_{N\to\infty}\left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}}(2\pi)^{\frac{N-1}{2}}\left[\det(\mathbf{A})\right]^{-\frac{1}{2}}\exp\left(\frac{1}{2}\mathbf{J}^T\mathbf{A}^{-1}\mathbf{J}\right)e^{\frac{im}{2\hbar\epsilon}(x_0-x_N)^2}. \tag{68}$$

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 (68) gives

$$\boxed{\langle x_N|U(t;0)|x_0\rangle = \sqrt{\tfrac{m}{2\pi i\hbar t}}e^{\frac{im}{2\hbar t}(x_0-x_N)^2}.} \tag{69}$$

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

$$\begin{aligned}\langle x_N|U(t;0)|x_0\rangle &= \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\langle x_N|e^{-i\frac{\hat{p}^2t}{2m\hbar}}|p\rangle\langle p|x_0\rangle = \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}e^{-i\frac{p^2t}{2m\hbar}+i\frac{p(x_0-x_N)}{\hbar}}\\ &= \sqrt{\frac{m}{2\pi i\hbar t}}e^{\frac{im}{2\hbar t}(x_0-x_N)^2}.\end{aligned} \tag{70}$$

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

$$f(z_0) = f(z_N) = 0. \tag{71}$$

The Laplace operator D acts on these functions as

$$Df \equiv \frac{d^2f(z)}{dz^2}. \tag{72}$$

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

$$z_n = z_0 + n a_0 \ , \quad n = 1, \ldots, N-1 \tag{73}$$

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

$$f(z) \to \mathbf{f} = (f(z_1), \ldots, f(z_{N-1})). \tag{74}$$

Recalling that

$$\frac{d^2 f}{dz^2}(z) = \lim_{a_0 \to 0} \frac{f(z+a_0) + f(z-a_0) - 2f(z)}{a_0^2} \ , \tag{75}$$

we conclude that the Lapacian is discretized as follows

$$Df \to a_0^{-2} \mathbf{\Delta f} \ , \tag{76}$$

where

$$\Delta_{jk} = \delta_{j,k+1} + \delta_{j,k-1} - 2\delta_{j,k}. \tag{77}$$

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

$$\mathbf{\Delta a}_n = \lambda_n \mathbf{a}_n, \quad n = 1, \ldots, N-1 \tag{78}$$

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

$$a_{n,j+1} + a_{n,j-1} - (2 + \lambda_n) a_{n,j} = 0. \tag{79}$$

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

$$a_{n,j} = C_n \sin\left(\frac{\pi n j}{N}\right). \tag{80}$$

Substituting this in to (79) gives

$$\lambda_n = 2\cos\left(\frac{\pi n}{N}\right) - 2 \ , \quad n = 1, \ldots, N-1. \tag{81}$$

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

$$\mathbf{a}_n = \frac{1}{\sqrt{\sum_{j=1}^{N-1} \sin^2\left(\frac{\pi n j}{N}\right)}} \begin{pmatrix} \sin\left(\frac{\pi n}{N}\right) \\ \sin\left(\frac{2\pi n}{N}\right) \\ \vdots \\ \sin\left(\frac{\pi(N-1)n}{N}\right). \end{pmatrix} = \sqrt{\frac{2}{N}} \begin{pmatrix} \sin\left(\frac{\pi n}{N}\right) \\ \sin\left(\frac{2\pi n}{N}\right) \\ \vdots \\ \sin\left(\frac{\pi(N-1)n}{N}\right). \end{pmatrix} \tag{82}$$

---

3 Path Integrals in Quantum Statistical Mechanics

An important quantity in Statistical Mechanics is the *partition function*

$$Z(\beta) = \mathrm{Tr}\left[e^{-\beta H}\right], \tag{83}$$

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

$$\beta = \frac{1}{k_B T}. \tag{84}$$

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

$$\langle \mathcal{O} \rangle_\beta = \frac{1}{Z(\beta)} \mathrm{Tr} \left[e^{-\beta H} \mathcal{O} \right]. \tag{85}$$

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

$$\begin{aligned} \langle \mathcal{O} \rangle_\beta &= \frac{1}{Z(\beta)} \sum_n e^{-\beta E_n} \langle n|\mathcal{O}|n\rangle \ , \\ Z(\beta) &= \sum_n e^{-\beta E_n}. \end{aligned} \tag{86}$$

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

$$\lim_{T\to 0} \langle \mathcal{O} \rangle_\beta = \langle 0|\mathcal{O}|0\rangle \ , \tag{87}$$

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

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}), \tag{88}$$

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

$$Z(\beta) = \int dx \langle x|e^{-\beta H}|x\rangle = \int dx \int dx' \ \langle x|x'\rangle \ \langle x'|e^{-\beta H}|x\rangle. \tag{89}$$

Here

$$\langle x'|e^{-\beta H}|x\rangle \tag{90}$$

is very similar to the propagator

$$\langle x'|e^{-\frac{i(t-t_0)}{\hbar} H}|x\rangle. \tag{91}$$

Formally (90) 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

$$\boxed{\langle x_N|e^{-\beta H}|x_0\rangle = \lim_{N\to\infty} \left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}} \int dx_1 \dots dx_{N-1} \exp\left(-\frac{\epsilon}{\hbar} \sum_{n=0}^{N-1} \frac{m}{2} \left(\frac{x_{n+1}-x_n}{\epsilon} \right)^2 + V(x_n) \right)} \ , \tag{92}$$

where now

$$\epsilon = \frac{\hbar\beta}{N}. \tag{93}$$

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

$$x(\tau_n) = x_n \ , \quad \tau_n = n\epsilon. \tag{94}$$

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

$$\boxed{\langle x_N|e^{-\beta H}|x_0\rangle = \mathcal{N} \int \mathcal{D}x(\tau) \ e^{-\frac{1}{\hbar} S_E[x(\tau)]},} \tag{95}$$

where S_E is called *Euclidean action*

$$S_E[x(\tau)] = \int_0^{\hbar\beta} d\tau \left[\frac{m}{2} \left(\frac{dx}{d\tau} \right)^2 + V(x) \right]. \tag{96}$$

Substituting (95) into the expression for the partition function we find that

$$\boxed{Z(\beta) = \mathcal{N} \int \mathcal{D}x(\tau)\ e^{-\frac{1}{\hbar} S_E[x(\tau)]},} \tag{97}$$

where we integrate over all *periodic paths*

$$x(\hbar\beta) = x(0). \tag{98}$$

The restriction to periodic paths arises because $Z(\beta)$ is a trace.

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

We now consider the simple harmonic oscillator

$$H = \frac{\hat{p}^2}{2m} + \frac{\kappa}{2}\hat{x}^2. \tag{99}$$

Let us work out the averages of powers of the position operator

$$\langle \hat{x}^n \rangle_\beta = \frac{\int dx\ \langle x|e^{-\beta H}\hat{x}^n|x\rangle}{\int dx \langle x|e^{-\beta H}|x\rangle} = \frac{\int dx\ x^n\ \langle x|e^{-\beta H}|x\rangle}{\int dx \langle x|e^{-\beta H}|x\rangle}. \tag{100}$$

We have

$$\langle x|e^{-\beta H}|x\rangle = \mathcal{N} \int \mathcal{D}x(\tau)\ e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + \frac{\kappa}{2}x^2\right]}, \tag{101}$$

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

$$-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + \frac{\kappa}{2}x^2\right] = -\frac{1}{2}\int_0^{\hbar\beta} d\tau\ x(\tau)\hat{D}x(\tau)\ , \tag{102}$$

where

$$\hat{D} = -\frac{m}{\hbar}\frac{d^2}{d\tau^2} + \frac{\kappa}{\hbar}. \tag{103}$$

We now define the *generating functional*

$$W[J] \equiv \mathcal{N} \int \mathcal{D}x(\tau)\ e^{-\frac{1}{2}\int_0^{\hbar\beta} d\tau \left[x(\tau)\hat{D}x(\tau) - 2J(\tau)x(\tau)\right]}. \tag{104}$$

Here the functions $J(\tau)$ are called *sources*. The point of the definition (104) is that we can obtain $\langle \hat{x}^n \rangle_\beta$ by taking functional derivatives

$$\langle \hat{x}^n \rangle_\beta = \frac{1}{W[0]}\frac{\delta}{\delta J(0)} \cdots \frac{\delta}{\delta J(0)}\bigg|_{J=0} W[J]. \tag{105}$$

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. We define the Green's function of the differential operator $\hat{D}_\tau$ in the usual way

$$\hat{D}_\tau G(\tau - \tau') = \delta(\tau - \tau')\ , \quad G(0) = G(\beta\hbar). \tag{106}$$

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

$$y(\tau) = x(\tau) - \int d\tau'\ G(\tau - \tau')J(\tau'). \tag{107}$$

We see that

$$\begin{aligned}\int d\tau\ y(\tau)\hat{D}_\tau y(\tau) &= \int d\tau\ x(\tau)\hat{D}_\tau x(\tau) + \int d\tau d\tau' d\tau''\ G(\tau-\tau')J(\tau')\hat{D}_\tau G(\tau-\tau'')J(\tau'') \\ &\quad - \int d\tau d\tau' \left[x(\tau)\hat{D}_\tau G(\tau-\tau')J(\tau') + G(\tau-\tau')J(\tau')\hat{D}_\tau x(\tau)\right] \\ &= \int d\tau\ x(\tau)\hat{D}_\tau x(\tau) + \int d\tau d\tau'\ G(\tau-\tau')J(\tau')J(\tau) - 2\int d\tau\ x(\tau)J(\tau)\ , \quad (108)\end{aligned}$$

where in the last step we have used (106) and integrated by parts twice to simplify the last term in the second line ($\int d\tau d\tau'\ G(\tau-\tau')J(\tau')\hat{D}_\tau x(\tau) = \int d\tau d\tau'\ x(\tau)\ \hat{D}_\tau G(\tau-\tau')J(\tau')$). The upshot is that

$$\int d\tau\ x(\tau)\hat{D}_\tau x(\tau) - 2\int d\tau\ x(\tau)J(\tau) = \int d\tau\ y(\tau)\hat{D}_\tau y(\tau) - \int d\tau d\tau'\ J(\tau)G(\tau-\tau')J(\tau'). \quad (109)$$

On the other hand, the Jacobian of the change of variables (107) 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

$$\boxed{W[J] = W[0]\ e^{\frac{1}{2}\int d\tau d\tau'\ J(\tau)G(\tau-\tau')J(\tau')}.} \quad (110)$$

Now we are ready to calculate (105). The average position is zero

$$\langle\hat{x}\rangle_\beta = \frac{1}{W[0]}\frac{\delta}{\delta J(0)}\bigg|_{J=0} W[J] = \frac{1}{2}\int d\tau d\tau' \left[\delta(\tau)G(\tau-\tau')J(\tau') + J(\tau)G(\tau-\tau')\delta(\tau')\right] W[J]\bigg|_{J=0} = 0. \quad (111)$$

Here we have used that

$$\frac{\delta J(\tau)}{\delta J(\tau')} = \delta(\tau-\tau'). \quad (112)$$

The expression (111) 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

$$\langle\hat{x}^{2n+1}\rangle_\beta = 0. \quad (113)$$

Next we turn to

$$\begin{aligned}\langle\hat{x}^2\rangle_\beta &= \frac{1}{W[0]}\frac{\delta}{\delta J(0)}\frac{\delta}{\delta J(0)}\bigg|_{J=0} W[J] \\ &= \frac{1}{W[0]}\frac{\delta}{\delta J(0)}\bigg|_{J=0}\frac{1}{2}\int d\tau d\tau' \left[\delta(\tau)G(\tau-\tau')J(\tau') + J(\tau)G(\tau-\tau')\delta(\tau')\right] W[J] = G(0). \quad (114)\end{aligned}$$

So the means square deviation of the oscillator's position is equal to the Green's function evaluated at zero. To determine $G(\tau)$ we need to solve the differential equation (106). As $G(0) = G(\beta\hbar)$ we are dealing with a periodic function and therefore may employ a Fourier expansion

$$G(\tau) = \frac{1}{\sqrt{\beta\hbar}}\sum_{n=-\infty}^{\infty} g_n e^{2\pi i n\tau/\beta\hbar}. \quad (115)$$

Substituting this into the differential equation gives

$$\hat{D}G(\tau) = \frac{1}{\sqrt{\beta\hbar}}\sum_{n=-\infty}^{\infty} g_n e^{2\pi i n\tau/\beta\hbar}\left[\frac{m}{\hbar}\left(\frac{2\pi n}{\beta\hbar}\right)^2 + \frac{\kappa}{\hbar}\right] = \delta(\tau). \quad (116)$$

Taking the integral $\int_0^{\hbar\beta} d\tau e^{-2\pi i k\tau/\hbar\beta}$ on both sides fixes the Fourier coefficients and we obtain

$$G(\tau) = \frac{1}{\beta\kappa} \sum_{n=-\infty}^{\infty} \frac{1}{1 + \left(\frac{2\pi n}{\beta\hbar\omega}\right)^2} e^{2\pi i n\tau\beta\hbar} , \tag{117}$$

where $\omega = \sqrt{\kappa/m}$. Setting $\tau = 0$ gives the desired result

$$G(0) = \frac{\hbar\omega}{2\kappa \tanh\left(\beta\hbar\omega/2\right)} = \frac{\hbar\omega}{\kappa}\left[\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2}\right]. \tag{118}$$

Using equipartition

$$\langle H\rangle_\beta = \langle T\rangle_\beta + \langle V\rangle_\beta = 2\langle V\rangle_\beta = \kappa\langle\hat{x}^2\rangle_\beta, \tag{119}$$

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

$$\langle H\rangle_\beta = \hbar\omega\left[\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2}\right]. \tag{120}$$

Recalling that

$$H = \hbar\omega\big(\hat{n} + \frac{1}{2}\big), \tag{121}$$

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

$$\langle\hat{n}\rangle_\beta = \frac{1}{e^{\beta\hbar\omega} - 1}. \tag{122}$$

3.2 Correlation Functions

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

$$\frac{1}{W[0]}\prod_{j=1}^{n}\frac{\delta}{\delta J(\tau_j)}\bigg|_{J=0} W[J] = \frac{\mathcal{N}}{W[0]}\int \mathcal{D}x(\tau)\prod_{j=1}^{n} x(\tau_j)\; e^{-\frac{1}{2}\int_0^{\hbar\beta} d\tau\; x(\tau)\hat{D}x(\tau)} . \tag{123}$$

What is their significance? Graphically, the path integral in (123) is represented in Fig. 2. It consists of

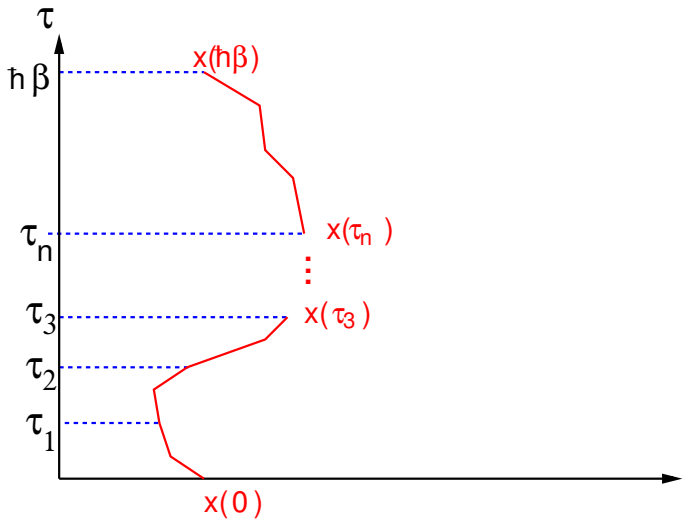


Figure 2: Path integral corresponding to (123).

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

$$\langle x(\tau_1)|e^{-H\tau_1/\hbar}|x(0)\rangle. \tag{124}$$

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

$$\langle x(\tau_2)|e^{-H(\tau_2-\tau_1)/\hbar}\hat{x}|x(\tau_1)\rangle. \tag{125}$$

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

$$\left[\prod_{j=1}^{n}\langle x(\tau_{j+1})|e^{-H(\tau_{j+1}-\tau_j)/\hbar}\hat{x}|x(\tau_j)\rangle\right]\langle x(\tau_1)|e^{-H\tau_1/\hbar}|x(0)\rangle\ , \tag{126}$$

where $\tau_{n+1} = \hbar\beta$. Finally, in order to represent the full path integral (123) 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

$$\begin{aligned}\frac{1}{Z(\beta)}\int dx(0)\langle x(0)|e^{-H(\beta-\tau_n)/\hbar}\hat{x}e^{-H(\tau_n-\tau_{n-1})/\hbar}\hat{x}\ldots\hat{x}e^{-H(\tau_2-\tau_1)/\hbar}\hat{x}e^{-H\tau_1/\hbar}|x(0)\rangle \\ = \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}\bar{x}(\tau_1)\bar{x}(\tau_2)\ldots\bar{x}(\tau_n)\right],\end{aligned} \tag{127}$$

where we have defined operators

$$\bar{x}(\tau_j) = e^{H\tau_j/\hbar}\hat{x}e^{-H\tau_j/\hbar}. \tag{128}$$

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 (123) 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

$$T_\tau\bar{x}(\tau_1)\bar{x}(\tau_2) = \theta(\tau_1-\tau_2)\bar{x}(\tau_1)\bar{x}(\tau_2) + \theta(\tau_2-\tau_1)\bar{x}(\tau_2)\bar{x}(\tau_1), \tag{129}$$

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

$$\boxed{\frac{1}{W[0]}\prod_{j=1}^{n}\frac{\delta}{\delta J(\tau_j)}\bigg|_{J=0}W[J] = \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}T_\tau\bar{x}(\tau_1)\bar{x}(\tau_2)\ldots\bar{x}(\tau_n)\right].} \tag{130}$$

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

$$\hat{x}(t) \equiv e^{\frac{it}{\hbar}H}\hat{x}e^{-\frac{it}{\hbar}H}. \tag{131}$$

The quantities that we get from (130) after analytic continuation are called *n-point correlation functions*

$$\boxed{\langle T\hat{x}(t_1)\hat{x}(t_2)\ldots\hat{x}(t_n)\rangle_\beta \equiv \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}T\hat{x}(t_1)\hat{x}(t_2)\ldots\hat{x}(t_n)\right].} \tag{132}$$

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.

3.2.1 Wick's Theorem

Recalling that

$$W[J] = W[0]\ e^{\frac{1}{2}\int d\tau d\tau'\ J(\tau)G(\tau-\tau')J(\tau')}, \tag{133}$$

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

$$\frac{1}{W[0]}\prod_{j=1}^{n}\frac{\delta}{\delta J(\tau_j)}\bigg|_{J=0} W[J] = \sum_{P(1,\ldots,n)} G(\tau_{P_1}-\tau_{P_2})\ldots G(\tau_{P_{n-1}}-\tau_{P_n})\ . \tag{134}$$

Here the sum is over all possible pairings of $\{1,2,\ldots,n\}$ and $G(\tau)$ is the Green's function (117). In particular we have

$$\langle T_\tau \bar{x}(\tau_1)\bar{x}(\tau_2)\rangle_\beta = G(\tau_1-\tau_2). \tag{135}$$

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.*

3.3 Perturbation Theory and Feynman Diagrams

Let us now consider the anharmonic oscillator

$$H = \frac{\hat{p}^2}{2m} + \frac{\kappa}{2}\hat{x}^2 + \frac{\lambda}{4!}\hat{x}^4. \tag{136}$$

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

$$W_\lambda[J] = \mathcal{N}\int \mathcal{D}x(\tau)\ e^{-\frac{1}{2}\int_0^{\hbar\beta} d\tau\left[x(\tau)\hat{D}x(\tau)-2J(\tau)x(\tau)\right]-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau\ x^4(\tau)}. \tag{137}$$

The partition function is

$$Z_\lambda(\beta) = W_\lambda[0]\ . \tag{138}$$

The idea is to expand (137) perturbatively in powers of λ

$$\begin{aligned}
W_\lambda[J] &= \mathcal{N}\int \mathcal{D}x(\tau)\ \left[1-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau'\ x^4(\tau')+\ldots\right] e^{-\frac{1}{2}\int_0^{\hbar\beta} d\tau\left[x(\tau)\hat{D}x(\tau)-2J(\tau)x(\tau)\right]} \\
&= \mathcal{N}\int \mathcal{D}x(\tau)\ \left[1-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau'\ \left[\frac{\delta}{\delta J(\tau')}\right]^4+\ldots\right] e^{-\frac{1}{2}\int_0^{\hbar\beta} d\tau\left[x(\tau)\hat{D}x(\tau)-2J(\tau)x(\tau)\right]} \\
&= \mathcal{N}\int \mathcal{D}x(\tau)\ e^{-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau'\ \left[\frac{\delta}{\delta J(\tau')}\right]^4} e^{-\frac{1}{2}\int_0^{\hbar\beta} d\tau\left[x(\tau)\hat{D}x(\tau)-2J(\tau)x(\tau)\right]} \\
&= e^{-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau'\ \left[\frac{\delta}{\delta J(\tau')}\right]^4} W_0[J].
\end{aligned} \tag{139}$$

We already know $W_0[J]$

$$W_0[J] = W_0[0]\ e^{\frac{1}{2}\int d\tau d\tau'\ J(\tau)G(\tau-\tau')J(\tau')}, \tag{140}$$

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

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

3.3.1 Partition Function of the anharmonic oscillator

By virtue of (138) the perturbation expansion for $Z_\lambda(\beta)$ is

$$\begin{aligned} Z_\lambda(\beta) &= e^{-\frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau' \left[\frac{\delta}{\delta J(\tau')}\right]^4} W_0[J]\Big|_{J=0} = Z_0(\beta) - \frac{\lambda}{4!\hbar}\int_0^{\hbar\beta} d\tau' \left[\frac{\delta}{\delta J(\tau')}\right]^4\Big|_{J=0} W_0[J] \\ &\quad -\frac{1}{2}\left[\frac{\lambda}{4!\hbar}\right]^2 \int_0^{\hbar\beta} d\tau' d\tau'' \left[\frac{\delta}{\delta J(\tau')}\right]^4 \left[\frac{\delta}{\delta J(\tau'')}\right]^4\Big|_{J=0} W_0[J] + \ldots \\ &= Z_0(\beta)\left[1 + \lambda\gamma_1(\beta) + \lambda^2\gamma_2(\beta) + \ldots\right]. \end{aligned} \tag{141}$$

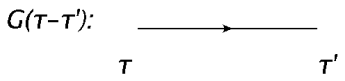
1. *First order perturbation theory.*

   Carrying out the functional derivatives gives

$$\lambda\gamma_1(\beta) = -\frac{\lambda}{8\hbar}\int_0^{\hbar\beta} d\tau' \ [G(\tau-\tau)]^2 = -\frac{\lambda\beta}{8}\left[G(0)\right]^2. \tag{142}$$

   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

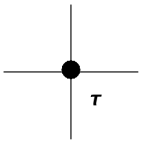


Figure 3: Graphical representation of the interaction vertex.

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

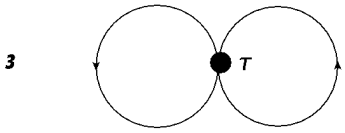


Figure 4: Feynman diagram for the 1st order perturbative contribution to the partition function.

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

$$\lambda^2\gamma_2(\beta) = \frac{1}{2}\left(\frac{\lambda}{4!\hbar}\right)^2 72\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\; G(\tau-\tau)G^2(\tau-\tau')G(\tau'-\tau')$$
$$+ \frac{1}{2}\left(\frac{\lambda}{4!\hbar}\right)^2 24\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\; G^4(\tau-\tau')$$
$$+ \frac{1}{2}\left(\frac{\lambda}{4!\hbar}\right)^2 9\left[\int_0^{\hbar\beta} d\tau G^2(\tau-\tau)\right]^2 . \qquad (143)$$

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

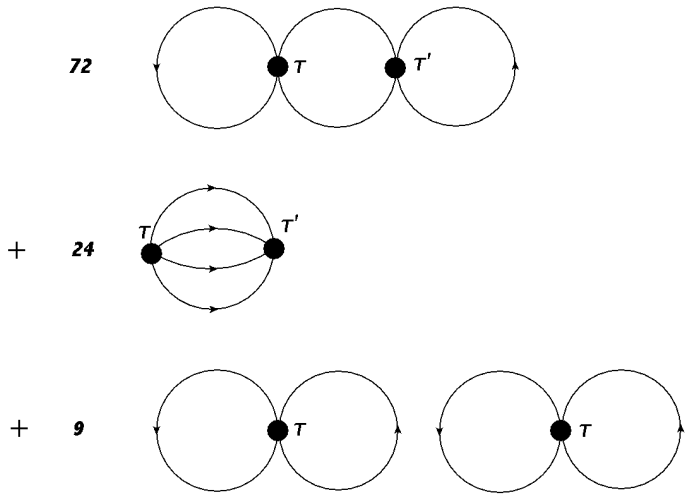


Figure 5: Feynman diagram for the 2nd order perturbative contribution to the partition function.

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

$$W[J] = W[0]e^{\frac{1}{2}J_1G_{12}J_2} = W[0]\left[1+\frac{1}{2}J_1G_{12}J_2+\frac{1}{2^3}J_1G_{12}J_2J_3G_{34}J_4+\ldots\right]. \qquad (144)$$

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

$$\frac{1}{2^3} \qquad (145)$$

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!

3.3.2 Green's Function of the anharmonic oscillator

Homework problem?

Part II
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*.

4 Second Quantization

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

4.1 Systems of Independent Particles

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

$$H = \sum_{j=1}^{N} H_j \tag{146}$$

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

$$H_j = \frac{\hat{\mathbf{p}}_j^2}{2m} + V(\hat{\mathbf{r}}_j) = -\frac{\hbar^2}{2m}\nabla_j^2 + V(\hat{\mathbf{r}}_j). \tag{147}$$

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

  $$H_j|\phi_l\rangle = E_l|\phi\rangle \ . \tag{148}$$

  The corresponding wave functions are

  $$\phi_l(\mathbf{r}_j) = \langle \mathbf{r}_j|\phi_l\rangle. \tag{149}$$

  The eigenstates form an orthonormal set

  $$\langle\phi_l|\phi_m\rangle = \delta_{l,m} = \int d^D\mathbf{r}_j \ \phi_l^*(\mathbf{r}_j)\phi_m(\mathbf{r}_j). \tag{150}$$

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

$$\left(\sum_{j=1}^{N} H_j\right) \phi_{l_1}(\mathbf{r}_1)\phi_{l_2}(\mathbf{r}_2)\dots\phi_{l_N}(\mathbf{r}_N) = \left(\sum_{j=1}^{N} E_{l_j}\right) \phi_{l_1}(\mathbf{r}_1)\phi_{l_2}(\mathbf{r}_2)\dots\phi_{l_N}(\mathbf{r}_N) \ . \tag{151}$$

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

$$|l_1\rangle \otimes |l_2\rangle \otimes \cdots \otimes |l_N\rangle. \tag{152}$$

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

$$\psi_{\pm}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{2}\left[\phi_l(\mathbf{r}_1)\phi_m(\mathbf{r}_2) \pm \phi_l(\mathbf{r}_2)\phi_m(\mathbf{r}_1)\right]. \tag{153}$$

Generally we require

$$\psi(\dots, \mathbf{r}_i, \dots, \mathbf{r}_j, \dots) = \pm\psi(\dots, \mathbf{r}_j, \dots, \mathbf{r}_i, \dots) \ , \tag{154}$$

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

$$\boxed{\psi_{l_1\dots l_N}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \mathcal{N} \sum_{P\in S_N} (\pm 1)^{|P|} \phi_{l_{P_1}}(\mathbf{r}_1)\dots\phi_{l_{P_N}}(\mathbf{r}_N),} \tag{155}$$

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

$$\mathcal{N} = \frac{1}{\sqrt{N! n_1! n_2! \dots}} \ , \tag{156}$$

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*

$$\psi_{l_1\dots l_N}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \phi_{l_1}(\mathbf{r}_1) & \dots & \phi_{l_1}(\mathbf{r}_N) \\ \vdots & & \vdots \\ \phi_{l_N}(\mathbf{r}_1) & \dots & \phi_{l_N}(\mathbf{r}_N) \end{pmatrix}. \tag{157}$$

The states corresponding to (155) are

$$\boxed{|l_1, \dots, l_N\rangle = \mathcal{N} \sum_{P\in S_N} (\pm 1)^{|P|} |l_{P_1}\rangle \otimes \cdots \otimes |l_{P_N}\rangle \ .} \tag{158}$$

4.1.1 Occupation Number Representation

By construction the states have the symmetry

$$|l_{Q_1} \dots l_{Q_N}\rangle = \pm|l_1 \dots l_N\rangle \ , \tag{159}$$

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

$$|\underbrace{1\dots1}_{n_1}\underbrace{2\dots2}_{n_2}\underbrace{3\dots3}_{n_3}4\dots\rangle \equiv |n_1 n_2 n_3 \dots\rangle. \tag{160}$$

In (160) 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 (160) 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

$$\langle m_1 m_2 m_3 \dots | n_1 n_2 n_3 \dots \rangle = \prod_j \delta_{n_j, m_j} \ , \tag{161}$$

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

4.2 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 $\sum_j n_j = N$.

4.2.1 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

$$\boxed{c_l^\dagger | n_1 n_2 \dots \rangle = \begin{cases} 0 & \text{if } n_l = 1 \text{ for fermions} \\ \sqrt{n_l + 1} (\pm 1)^{\sum_{j=1}^{l-1} n_j} | n_1 n_2 \dots n_l + 1 \dots \rangle & \text{else.} \end{cases}} \tag{162}$$

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

- particle annihilation operators with quantum number l

$$\boxed{c_l | n_1 n_2 \dots \rangle = \sqrt{n_l} (\pm 1)^{\sum_{j=1}^{l-1} n_j} | n_1 n_2 \dots n_l - 1 \dots \rangle \ .} \tag{163}$$

We note that (163) follows from (162) by

$$\langle m_1 m_2 \dots | c_l^\dagger | n_1 n_2 \dots \rangle^* = \langle n_1 n_2 \dots | c_l | m_1 m_2 \dots \rangle \ . \tag{164}$$

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

$$\boxed{[c_l, c_m] = 0 = [c_l^\dagger, c_m^\dagger] \ , \quad [c_l, c_m^\dagger] = \delta_{l,m} \qquad \text{bosons,}} \tag{165}$$

$$\boxed{\{c_l, c_m\} = c_l c_m + c_m c_l = 0 = \{c_l^\dagger, c_m^\dagger\} \ , \quad \{c_l, c_m^\dagger\} = \delta_{l,m} \qquad \text{fermions.}} \tag{166}$$

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

Let us see how to prove these: let us consider the fermionic case and take $l > m$. Then

$$\begin{aligned} c_l^\dagger c_m |\dots n_l \dots n_m \dots\rangle &= c_l^\dagger \sqrt{n_m} (-1)^{\sum_{j=1}^{m-1} n_j} |\dots n_l \dots n_m - 1 \dots\rangle \\ &= \sqrt{n_l + 1}\sqrt{n_m} (-1)^{\sum_{j=l+1}^{m-1} n_j} |\dots n_l + 1 \dots n_m - 1 \dots\rangle. \end{aligned} \tag{167}$$

Similarly we have

$$c_m c_l^\dagger |\dots n_l \dots n_m \dots\rangle = \sqrt{n_l + 1}\sqrt{n_m} (-1)^{1+\sum_{j=l+1}^{m-1} n_j} |\dots n_l + 1 \dots n_m - 1 \dots\rangle. \tag{168}$$

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

$$\{c_l^\dagger, c_m\} |n_1 n_2 \dots\rangle = 0 \ , \qquad \text{if } l > m. \tag{169}$$

This implies that

$$\{c_l^\dagger, c_m\} = 0 \ , \qquad \text{if } l > m. \tag{170}$$

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

$$c_l^\dagger c_l |\dots n_l \dots n_m \dots\rangle = c_l^\dagger \sqrt{n_l} (-1)^{\sum_{j=1}^{l-1} n_j} |\dots n_l - 1 \dots\rangle = n_l |\dots n_l \dots\rangle. \tag{171}$$

$$\begin{aligned} c_l c_l^\dagger |\dots n_l \dots\rangle &= \begin{cases} c_l \sqrt{n_l + 1} (-1)^{\sum_{j=1}^{l-1} n_j} |\dots n_l + 1 \dots\rangle & \text{if } n_l = 0 \ , \\ 0 & \text{if } n_l = 1 \ , \end{cases} \\ &= \begin{cases} |\dots n_l \dots\rangle & \text{if } n_l = 0 \ , \\ 0 & \text{if } n_l = 1 \ , \end{cases} \end{aligned} \tag{172}$$

Combining these we find that

$$\{c_l^\dagger, c_l\} |\dots n_l \dots\rangle = |\dots n_l \dots\rangle \ , \tag{173}$$

and as the states $|\dots n_l \dots\rangle$ form a basis this implies (here 1 really means 1 times the identity operator $\mathbf{1}$).

$$\{c_l^\dagger, c_l\} = 1. \tag{174}$$

4.2.2 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)
$$|0\rangle. \tag{175}$$

- Single-particle states
$$|0 \dots 0 \underbrace{1}_{l} 0 \dots\rangle = c_l^\dagger |0\rangle \ . \tag{176}$$

- N-particle states
$$|n_1 n_2 \dots\rangle = \prod_j \frac{1}{\sqrt{n_j!}} \left(c_j^\dagger\right)^{n_j} |0\rangle \ . \tag{177}$$

4.2.3 Change of Basis

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

$$\boxed{\text{single-particle states } |l\rangle} \longrightarrow \boxed{\text{N-particle states } |n_1 n_2 \dots\rangle} \longrightarrow \boxed{\text{Fock Space}}. \tag{178}$$

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

$$\{|l\rangle\} \longrightarrow \{|\alpha\rangle\} \ , \tag{179}$$

where

$$|\alpha\rangle = \sum_l \underbrace{\langle l|\alpha\rangle}_{U_{l\alpha}} \ |l\rangle. \tag{180}$$

By construction

$$\sum_\alpha U_{l\alpha} U^\dagger_{\alpha m} = \sum_\alpha \langle l|\alpha\rangle\langle\alpha|m\rangle = \langle l|m\rangle = \delta_{lm}. \tag{181}$$

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

$$\begin{aligned} |l\rangle &= c_l^\dagger|0\rangle \ , \\ |\alpha\rangle &= d_\alpha^\dagger|0\rangle \ . \end{aligned} \tag{182}$$

On the other hand we have

$$|\alpha\rangle = \sum_l U_{l\alpha}|l\rangle = \sum_l U_{l\alpha} c_l^\dagger|0\rangle. \tag{183}$$

This suggests that we take

$$\boxed{d_\alpha^\dagger = \sum_l U_{l\alpha} c_l^\dagger,} \tag{184}$$

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

$$\boxed{d_\alpha = \sum_l U^\dagger_{\alpha l} c_l.} \tag{185}$$

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

$$\{d_\alpha, d_\beta^\dagger\} = \sum_{l,m} U^\dagger_{\alpha l} U_{m\beta} \underbrace{\{c_l, c_m^\dagger\}}_{\delta_{l,m}} = \sum_l U^\dagger_{\alpha l} U_{l\beta} = (U^\dagger U)_{\alpha\beta} = \delta_{\alpha,\beta}. \tag{186}$$

4.3 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.

4.3.1 Occupation number operators

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

$$\hat{n}_l \equiv c_l^\dagger c_l. \tag{187}$$

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

$$\hat{n}_l|n_1 n_2 \dots\rangle = n_l|n_1 n_2 \dots\rangle. \tag{188}$$

4.3.2 Single-particle operators

Single-particle operators are of the form

$$\hat{O} = \sum_j \hat{o}_j \ , \tag{189}$$

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

$$\hat{T} = \sum_j \frac{\hat{p}_j^2}{2m} \ , \qquad \hat{V} = \sum_j V(\hat{x}_j). \tag{190}$$

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 $\hat{o}$

  $$\hat{o}|l\rangle = \lambda_l |l\rangle = \lambda_l c_l^\dagger |0\rangle. \tag{191}$$

  Then, when acting on an N-particle state (158), we have

  $$\hat{O}|l_1, l_2, \ldots, l_N\rangle = \left[\sum_{j=1}^N \lambda_j\right] |l_1, l_2, \ldots, l_N\rangle. \tag{192}$$

  This is readily translated into the occupation number representation

  $$\hat{O}|n_1 n_2 \ldots\rangle = \left[\sum_k n_k \lambda_k\right] |n_1 n_2 \ldots\rangle. \tag{193}$$

  As $|n_1 n_2 \ldots\rangle$ constitute a basis, this together with (188) imply that we can represent $\hat{O}$ in the form

  $$\hat{O} = \sum_k \lambda_k \hat{n}_k = \sum_k \lambda_k c_k^\dagger c_k. \tag{194}$$

- 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 (194) in the form

  $$\hat{O} = \sum_{k,k'} \langle k'|\hat{O}|k\rangle c_{k'}^\dagger c_k. \tag{195}$$

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

  $$c_k^\dagger = \sum_\alpha U_{\alpha k}^\dagger d_\alpha^\dagger. \tag{196}$$

  This gives

  $$\hat{O} = \sum_{\alpha,\beta} \underbrace{\sum_{k'} \left(\langle k'|U_{\alpha k'}^\dagger\right)}_{\langle\alpha|} \hat{O} \underbrace{\sum_k \left(U_{k\beta}|k\rangle\right)}_{|\beta\rangle} d_\alpha^\dagger d_\beta. \tag{197}$$

  where we have used that

  $$|k\rangle = \sum_\alpha U_{\alpha k}^\dagger |\alpha\rangle \ . \tag{198}$$

  This gives us the final result

  $$\boxed{\hat{O} = \sum_{\alpha,\beta} \langle\alpha|\hat{O}|\beta\rangle \ d_\alpha^\dagger d_\beta.} \tag{199}$$

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

$$\hat{\mathbf{P}}|\mathbf{k}\rangle = \mathbf{k}|\mathbf{k}\rangle \ , \quad \langle \mathbf{p}|\mathbf{k}\rangle = (2\pi\hbar)^3\delta^{(3)}(\mathbf{p}-\mathbf{k}). \tag{200}$$

These are shorthand notations for

$$\hat{P}_a|k_x,k_y,k_z\rangle = k_a|k_x,k_y,k_z\rangle \ , \quad a=x,y,z. \tag{201}$$

and

$$\langle p_x,p_y,p_z|k_x,k_y,k_z\rangle = (2\pi\hbar)^3\delta(k_x-p_x)\delta(k_y-p_y)\delta(k_z-p_z) \ . \tag{202}$$

Using our general result for representing single-particle operators in a Fock space built from their eigenstates (194) we have

$$\hat{\mathbf{P}} = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\mathbf{p}c^\dagger(\mathbf{p})c(\mathbf{p}) \ , \qquad [c^\dagger(\mathbf{k}),c(\mathbf{p})\} = (2\pi\hbar)^3\delta^{(3)}(\mathbf{p}-\mathbf{k}). \tag{203}$$

Here we have introduced a notation

$$[c^\dagger(\mathbf{k}),c(\mathbf{p})\} = \begin{cases} c^\dagger(\mathbf{k})c(\mathbf{p}) - c(\mathbf{p})c^\dagger(\mathbf{k}) & \text{for bosons} \\ c^\dagger(\mathbf{k})c(\mathbf{p}) + c(\mathbf{p})c^\dagger(\mathbf{k}) & \text{for fermions.} \end{cases} \tag{204}$$

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

$$\hat{\mathbf{X}}|\mathbf{x}\rangle = \mathbf{x}|\mathbf{x}\rangle \ , \quad \langle \mathbf{x}|\mathbf{x}'\rangle = \delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{205}$$

Our general formula (199) gives

$$\hat{\mathbf{P}} = \int d^3\mathbf{x}d^3\mathbf{x}' \ \langle \mathbf{x}'|\hat{\mathbf{P}}|\mathbf{x}\rangle c^\dagger(\mathbf{x}')c(\mathbf{x}) \ . \tag{206}$$

We can simplify this by noting that

$$\langle \mathbf{x}'|\hat{\mathbf{P}}|\mathbf{x}\rangle = -i\hbar\nabla_{\mathbf{x}'}\delta^{(3)}(\mathbf{x}-\mathbf{x}'), \tag{207}$$

which allows us to eliminate three of the integrals

$$\hat{\mathbf{P}} = \int d^3\mathbf{x}d^3\mathbf{x}' \left[-i\hbar\nabla_{\mathbf{x}'}\delta^{(3)}(\mathbf{x}-\mathbf{x}')\right] c^\dagger(\mathbf{x}')c(\mathbf{x}) = \int d^3\mathbf{x}c^\dagger(\mathbf{x})\left(-i\hbar\nabla_{\mathbf{x}}\right)c(\mathbf{x}). \tag{208}$$

2. Single-particle Hamiltonian:

$$H = \sum_{j=1}^{N}\frac{\hat{\mathbf{p}}_j^2}{2m} + V(\hat{\mathbf{x}}_j). \tag{209}$$

(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 (194) tells us that

$$H = \sum_l E_l c_l^\dagger c_l. \tag{210}$$

(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 (199)

$$H = \int d^3\mathbf{x} d^3\mathbf{x}' \ \langle \mathbf{x}'|H|\mathbf{x}\rangle \ c^\dagger(\mathbf{x}')c(\mathbf{x}). \tag{211}$$

Substituting (209) into (211) and using

$$\langle \mathbf{x}'|V(\hat{\mathbf{x}})|\mathbf{x}\rangle = V(\mathbf{x})\delta^{(3)}(\mathbf{x}-\mathbf{x}') \ , \quad \langle \mathbf{x}'|\hat{\mathbf{p}}^2|\mathbf{x}\rangle = -\hbar^2\nabla^2\delta^{(3)}(\mathbf{x}-\mathbf{x}') \ , \tag{212}$$

we arrive at the position representation

$$\boxed{H = \int d^3\mathbf{x} \ c^\dagger(\mathbf{x}) \left[-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{x})\right] c(\mathbf{x}).} \tag{213}$$

(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 (199)

$$H = \int \frac{d^3\mathbf{p} d^3\mathbf{p}'}{(2\pi\hbar)^6} \ \langle \mathbf{p}'|H|\mathbf{p}\rangle \ c^\dagger(\mathbf{p}')c(\mathbf{p}). \tag{214}$$

Matrix elements of the kinetic energy operator are simple

$$\langle \mathbf{p}'|\hat{\mathbf{p}}^2|\mathbf{p}\rangle = \mathbf{p}^2\langle \mathbf{p}'|\mathbf{p}\rangle = \mathbf{p}^2(2\pi\hbar)^3\delta^{(3)}(\mathbf{p}-\mathbf{p}'). \tag{215}$$

Matrix elements of the potential can be calcuated as follows

$$\begin{aligned} \langle \mathbf{p}'|\hat{V}|\mathbf{p}\rangle &= \int d^3\mathbf{x} d^3\mathbf{x}' \ \langle \mathbf{p}'|\mathbf{x}'\rangle\langle \mathbf{x}'|\hat{V}|\mathbf{x}\rangle\langle \mathbf{x}|\mathbf{p}\rangle = \int d^3\mathbf{x} d^3\mathbf{x}' \ \underbrace{\langle \mathbf{x}'|\hat{V}|\mathbf{x}\rangle}_{V(\mathbf{x})\delta^{(3)}(\mathbf{x}-\mathbf{x}')} \ e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}-\frac{i}{\hbar}\mathbf{p}'\cdot\mathbf{x}'} \\ &= \int d^3\mathbf{x} \ V(\mathbf{x})e^{\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{x}} = \tilde{V}(\mathbf{p}-\mathbf{p}'), \end{aligned} \tag{216}$$

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

$$\boxed{H = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} \ \frac{\mathbf{p}^2}{2m} c^\dagger(\mathbf{p})c(\mathbf{p}) + \int \frac{d^3\mathbf{p} d^3\mathbf{p}'}{(2\pi\hbar)^6} \ \tilde{V}(\mathbf{p}-\mathbf{p}')c^\dagger(\mathbf{p}')c(\mathbf{p}).} \tag{217}$$

4.3.3 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

$$\hat{V} = \sum_{i<j}^{N} V(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j). \tag{218}$$

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

$$\boxed{\hat{V} = \frac{1}{2}\int d^3\mathbf{r} d^3\mathbf{r}' \ c^\dagger(\mathbf{r})c^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')c(\mathbf{r}')c(\mathbf{r}).} \tag{219}$$

The derivation of (219) for fermions proceeds as follows. We start with our original representation of N-particle states (158)

$$|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \mathcal{N}\sum_{P\in S_N}(-1)^{|P|}|\mathbf{r}_1\rangle\otimes\ldots|\mathbf{r}_N\rangle\ . \tag{220}$$

Then

$$\hat{V}|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \sum_{i<j}V(\mathbf{r}_i,\mathbf{r}_j)|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \frac{1}{2}\sum_{i\neq j}V(\mathbf{r}_i,\mathbf{r}_j)|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle\ . \tag{221}$$

On the other hand we know that

$$|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \prod_{j=1}^{N}c^\dagger(\mathbf{r}_j)|0\rangle. \tag{222}$$

Now consider

$$c(\mathbf{r})|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = c(\mathbf{r})\prod_{j=1}^{N}c^\dagger(\mathbf{r}_j)|0\rangle = \{c(\mathbf{r}),\prod_{j=1}^{N}c^\dagger(\mathbf{r}_j)\}|0\rangle\ , \tag{223}$$

where is the last step we have used that $c(\mathbf{r})|0\rangle = 0$. The anticommutator is

$$\begin{aligned}\{c(\mathbf{r}),\prod_{j=1}^{N}c^\dagger(\mathbf{r}_j)\} &= \{c(\mathbf{r}),c^\dagger(\mathbf{r}_1)\}\prod_{j=2}^{N}c^\dagger(\mathbf{r}_j) - c^\dagger(\mathbf{r}_1)\{c(\mathbf{r}),c^\dagger(\mathbf{r}_2)\}\prod_{j=3}^{N}c^\dagger(\mathbf{r}_j)\\ &\quad +\ldots+\prod_{j=1}^{N-1}c^\dagger(\mathbf{r}_j)\{c(\mathbf{r}),c^\dagger(\mathbf{r}_N)\}.\end{aligned} \tag{224}$$

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

$$c(\mathbf{r})|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \sum_{n=1}^{N}(-1)^{n-1}\delta^{(3)}(\mathbf{r}-\mathbf{r}_n)\prod_{j\neq n}^{N}c^\dagger(\mathbf{r}_j)|0\rangle = \sum_{n=1}^{N}(-1)^{n-1}\delta^{(3)}(\mathbf{r}-\mathbf{r}_n)|\mathbf{r}_1\ldots\overbrace{\mathbf{r}_n}^{\text{missing}}\ldots\mathbf{r}_N\rangle. \tag{225}$$

Hence

$$\underbrace{c^\dagger(\mathbf{r}')c(\mathbf{r}')}_{\text{number op.}}c(\mathbf{r})|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \sum_{n=1}^{N}(-1)^{n-1}\delta^{(3)}(\mathbf{r}-\mathbf{r}_n)\sum_{m\neq n}^{N}\delta^{(3)}(\mathbf{r}'-\mathbf{r}_m)\ |\mathbf{r}_1\ldots\overbrace{\mathbf{r}_n}^{\text{missing}}\ldots\mathbf{r}_N\rangle, \tag{226}$$

and finally

$$c^\dagger(\mathbf{r})c^\dagger(\mathbf{r}')c(\mathbf{r}')c(\mathbf{r})|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \sum_{n=1}^{N}\delta^{(3)}(\mathbf{r}-\mathbf{r}_n)\sum_{m\neq n}^{N}\delta^{(3)}(\mathbf{r}'-\mathbf{r}_m)\ |\mathbf{r}_1\ldots\mathbf{r}_n\ldots\mathbf{r}_N\rangle. \tag{227}$$

This implies that

$$\frac{1}{2}\int d^3\mathbf{r}d^3\mathbf{r}'\ V(\mathbf{r},\mathbf{r}')\ c^\dagger(\mathbf{r})c^\dagger(\mathbf{r}')c(\mathbf{r}')c(\mathbf{r})|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle = \frac{1}{2}\sum_{n\neq m}V(\mathbf{r}_n,\mathbf{r}_m)|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle. \tag{228}$$

As $\{|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle\}$ form a basis, this establishes (219).

Using our formula for basis transformations (184)

$$c^\dagger(\mathbf{r}) = \sum_l\langle l|\mathbf{r}\rangle\ c_l^\dagger, \tag{229}$$

we can transform (219) into a general basis. We have

$$\hat{V} = \frac{1}{2}\sum_{ll'mm'}\int d^3\mathbf{r}d^3\mathbf{r}'\; V(\mathbf{r},\mathbf{r}')\langle l|\mathbf{r}\rangle\langle l'|\mathbf{r}'\rangle\langle \mathbf{r}'|m\rangle\langle \mathbf{r}|m'\rangle c_l^\dagger c_{l'}^\dagger c_m c_{m'}\ . \tag{230}$$

We can rewrite this by using that $\hat{V}|\mathbf{r}\rangle\otimes|\mathbf{r}'\rangle = V(\mathbf{r},\mathbf{r}')|\mathbf{r}\rangle\otimes|\mathbf{r}'\rangle$

$$\begin{aligned} V(\mathbf{r},\mathbf{r}')\langle l|\mathbf{r}\rangle\langle l'|\mathbf{r}'\rangle\langle \mathbf{r}'|m\rangle\langle \mathbf{r}|m'\rangle &= V(\mathbf{r},\mathbf{r}')\left[\langle l|\otimes\langle l'|\right]\left[|\mathbf{r}\rangle\otimes|\mathbf{r}'\rangle|\right]\left[\langle \mathbf{r}'|\otimes\langle \mathbf{r}|\right]\left[|m\rangle\otimes|m'\rangle|\right] \\ &= \left[\langle l|\otimes\langle l'|\right]\hat{V}\left[|\mathbf{r}\rangle\otimes|\mathbf{r}'\rangle|\right]\left[\langle \mathbf{r}'|\otimes\langle \mathbf{r}|\right]\left[|m\rangle\otimes|m'\rangle|\right] \end{aligned} \tag{231}$$

Now we use that

$$\int d^3\mathbf{r}d^3\mathbf{r}'\left[|\mathbf{r}\rangle\otimes|\mathbf{r}'\rangle\right]\left[\langle \mathbf{r}'|\otimes\langle \mathbf{r}|\right] = \mathbf{1} \tag{232}$$

to obtain

$$\hat{V} = \frac{1}{2}\sum_{ll'mm'}\left[\langle l|\otimes\langle l'|\right]|\hat{V}|\left[m\rangle\otimes|m'\rangle\right]c_l^\dagger c_{l'}^\dagger c_m c_{m'}\ . \tag{233}$$

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

$$|ll'\rangle = \frac{1}{\sqrt{2}}\left[|l\rangle\otimes|l'\rangle \pm |l'\rangle\otimes|l\rangle\right] \qquad (l\neq l'). \tag{234}$$

in the form

$$\boxed{\hat{V} = \sum_{ll'mm'}\langle ll'|\hat{V}|mm'\rangle c_l^\dagger c_{l'}^\dagger c_m c_{m'}\ .} \tag{235}$$

The representation (235) generalizes to arbitrary two-particle operators $\mathcal{O}$.

4.4 Lattice Models

These constitute a *very* important class of models in condensed matter physics. To see what these are about let us consider a crystal lattice, in which the ion cores are separated by a distance that is large compared to the Bohr radius of the valence electrons. In this *atomic limit* the electron wave functions are substantially different from zero only in close vicinity of the lattice sites $\mathbf{R}_n$, i.e. the positions of the ion cores (which we take to be constant for simplicity). It is convenient to use a basis of atomic eigenstates $|\psi_{\mathbf{R},n}\rangle$

5 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

$$c_\sigma^\dagger(\mathbf{p})\ , \quad \sigma = \uparrow,\downarrow\ . \tag{236}$$

They fulfil canonical anticommutation relations

$$\{c_\sigma(\mathbf{p}),c_\tau(\mathbf{k})\} = 0 = \{c_\sigma^\dagger(\mathbf{p}),c_\tau^\dagger(\mathbf{k})\}\ , \qquad \{c_\sigma(\mathbf{p}),c_\tau^\dagger(\mathbf{k})\} = \delta_{\sigma,\tau}(2\pi\hbar)^3\delta^{(3)}(\mathbf{k}-\mathbf{p}). \tag{237}$$

The Hamiltonian, in the grand canonical ensemble, is

$$H-\mu\hat{N} = \int\frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\underbrace{\left[\frac{\mathbf{p}^2}{2m}-\mu\right]}_{\epsilon(\mathbf{p})}\sum_{\sigma=\uparrow,\downarrow}c_\sigma^\dagger(\mathbf{p})c_\sigma(\mathbf{p}). \tag{238}$$

Here $\mu > 0$ is the chemical potential. As $c^\dagger_\sigma(\mathbf{p})c_\sigma(\mathbf{p}) = \hat{n}_\sigma(\mathbf{p})$ 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:

$$\begin{aligned}
\left[H - \mu\hat{N}\right]|0\rangle &= 0\ , \\
\left[H - \mu\hat{N}\right]c^\dagger_\sigma(\mathbf{p})|0\rangle &= \epsilon(\mathbf{p})\ c^\dagger_{\sigma_j}(\mathbf{p})|0\rangle\ , \\
\left[H - \mu\hat{N}\right]\prod_{j=1}^{n} c^\dagger_\sigma(\mathbf{p}_j)|0\rangle &= \left[\sum_{k=1}^{n}\epsilon(\mathbf{p}_k)\right]\prod_{j=1}^{n} c^\dagger_{\sigma_j}(\mathbf{p}_j)|0\rangle\ .
\end{aligned} \tag{239}$$

5.1 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

$$\hat{\mathbf{p}}\psi_{\mathbf{k}}(\mathbf{r}) = -i\hbar\nabla\psi_{\mathbf{k}}(\mathbf{r}) = \mathbf{k}\psi_{\mathbf{k}}(\mathbf{r}). \tag{240}$$

The solutions are plane waves

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{r}}. \tag{241}$$

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

$$\psi_{\mathbf{k}}(\mathbf{r} + L\mathbf{e}_a) = \psi_{\mathbf{k}}(\mathbf{r}) \quad \text{for } a = x, y, z, \tag{242}$$

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

$$e^{\frac{i}{\hbar}Lk_a} = 1 \Rightarrow k_a = \frac{2\pi\hbar n_a}{L}\ , \quad a = x, y, z. \tag{243}$$

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

$$\mathbf{k} = \frac{2\pi\hbar}{L}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} \tag{244}$$

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

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{L^{\frac{3}{2}}}e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{r}}. \tag{245}$$

Hence

$$\langle\mathbf{k}|\mathbf{k}'\rangle = \int d^3\mathbf{r}\psi^*_{\mathbf{k}}(\mathbf{r})\psi_{\mathbf{k}'}(\mathbf{r}) = \delta_{\mathbf{k},\mathbf{k}'}. \tag{246}$$

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

$$\{c_\sigma(\mathbf{p}), c_\tau(\mathbf{k})\} = 0 = \{c^\dagger_\sigma(\mathbf{p}), c^\dagger_\tau(\mathbf{k})\}\ , \qquad \{c^\dagger_\sigma(\mathbf{p}), c_\tau(\mathbf{k})\} = \delta_{\sigma,\tau}\delta_{\mathbf{k},\mathbf{p}}. \tag{247}$$

The Hamiltonian is

$$\boxed{H - \mu\hat{N} = \sum_{\mathbf{p}}\epsilon(\mathbf{p})\sum_{\sigma=\uparrow,\downarrow} c^\dagger_\sigma(\mathbf{p})c_\sigma(\mathbf{p}).} \tag{248}$$

We define a *Fermi momentum* by

$$\frac{p_F^2}{2m} = \mu. \tag{249}$$

5.1.1 Ground State

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

$$\boxed{|\mathrm{GS}\rangle = \prod_{|\mathbf{p}|<p_F,\sigma} c_\sigma^\dagger(\mathbf{p})|0\rangle.} \tag{250}$$

The ground state energy is

$$E_{\mathrm{GS}} = \sum_\sigma \sum_{|\mathbf{p}|<p_F} \epsilon(\mathbf{p}). \tag{251}$$

This is extensive (proportional to the volume) as expected. You can see the advantage of working in a finite volume: the product in (250) involves only a finite number of factors and the ground state energy is finite. The ground state momentum is

$$P_{\mathrm{GS}} = \sum_\sigma \sum_{|\mathbf{p}|<p_F} \mathbf{p} = 0. \tag{252}$$

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 $-\mathbf{p}$.

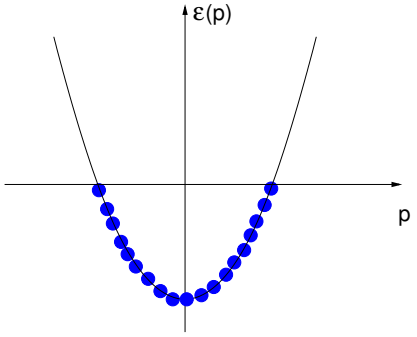


Figure 6: Ground state in the 1 dimensional case. Blue circles correspond to "filled" single-particle states.

5.1.2 Excitations

- Particle excitations

$$c_\sigma^\dagger(\mathbf{k})|\mathrm{GS}\rangle \qquad \text{with } |\mathbf{k}| > p_F. \tag{253}$$

  Their energies and momenta are

$$E = E_{\mathrm{GS}} + \epsilon(\mathbf{k}) > E_{\mathrm{GS}}\ , \quad \mathbf{P} = \mathbf{k}. \tag{254}$$

- Hole excitations

$$c_\sigma(\mathbf{k})|\mathrm{GS}\rangle \qquad \text{with } |\mathbf{k}| < p_F. \tag{255}$$

  Their energies and momenta are

$$E = E_{\mathrm{GS}} - \epsilon(\mathbf{k}) > E_{\mathrm{GS}}\ , \quad \mathbf{P} = -\mathbf{k}. \tag{256}$$

- Particle-hole excitations

$$c_\sigma^\dagger(\mathbf{k})c_\tau(\mathbf{p})|\mathrm{GS}\rangle \qquad \text{with } |\mathbf{k}| > p_F > |\mathbf{p}|. \tag{257}$$

  Their energies and momenta are

$$E = E_{\mathrm{GS}} + \epsilon(\mathbf{k}) - \epsilon(\mathbf{p}) > E_{\mathrm{GS}}\ , \quad \mathbf{P} = \mathbf{k} - \mathbf{p}. \tag{258}$$

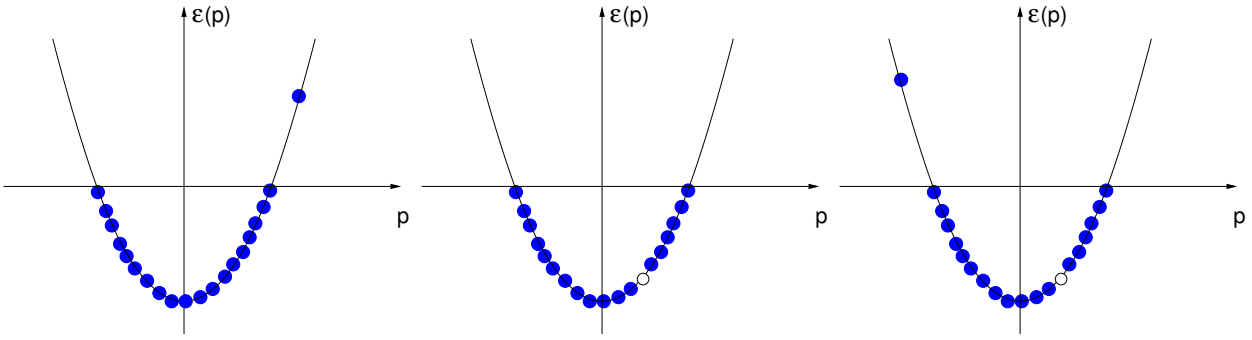


Figure 7: Some simple excited states: (a) particle (b) hole (c) particle-hole.

5.1.3 Density Correlations

Consider the single-particle operator

$$o = |\mathbf{r}\rangle\langle\mathbf{r}| \tag{259}$$

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

$$\rho(\mathbf{r}) = \sum_\sigma \int d^3\mathbf{r}' d^3\mathbf{r}'' \ \langle\mathbf{r}'|o|\mathbf{r}''\rangle \ c_\sigma^\dagger(\mathbf{r}')c_\sigma(\mathbf{r}'') = \sum_\sigma c_\sigma^\dagger(\mathbf{r})c_\sigma(\mathbf{r}). \tag{260}$$

1. One-point function.

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

   $$\langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle = \sum_\sigma \langle \mathrm{GS}|c_\sigma^\dagger(\mathbf{r})c_\sigma(\mathbf{r})|\mathrm{GS}\rangle. \tag{261}$$

   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 (185) that

   $$c_\sigma(\mathbf{r}) = \sum_{\mathbf{p}} \underbrace{\langle\mathbf{r}|\mathbf{p}\rangle}_{L^{-3/2}e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}} c_\sigma(\mathbf{p}). \tag{262}$$

   Substituting this as well as the analogous expression for the creation operator into (261), we obtain

   $$\langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle = \sum_\sigma \frac{1}{L^3} \sum_{\mathbf{p},\mathbf{p}'} e^{\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} \langle \mathrm{GS}|c_\sigma^\dagger(\mathbf{p}')c_\sigma(\mathbf{p})|\mathrm{GS}\rangle. \tag{263}$$

   For the expectation value $\langle \mathrm{GS}|c_\sigma^\dagger(\mathbf{p}')c_\sigma(\mathbf{p})|\mathrm{GS}\rangle$ to be non-zero, we must have that $c_\sigma^\dagger(\mathbf{p}')c_\sigma(\mathbf{p})|\mathrm{GS}\rangle$ 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). Hence

   $$\langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle = \sum_\sigma \frac{1}{L^3} \sum_{\mathbf{p},\mathbf{p}'} e^{\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} \delta_{\mathbf{p},\mathbf{p}'} \ \theta(p_F - |\mathbf{p}|) = \underbrace{2}_{\text{spin}} \frac{1}{L^3} \sum_{\mathbf{p}} \theta(p_F - |\mathbf{p}|) = \frac{N}{L}. \tag{264}$$

   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

$$\langle \mathrm{GS}|\rho(\mathbf{r})\rho(\mathbf{r}')|\mathrm{GS}\rangle = \sum_{\sigma,\sigma'} \frac{1}{L^6} \sum_{\mathbf{p},\mathbf{p}'} \sum_{\mathbf{k},\mathbf{k}'} e^{\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}} e^{\frac{i}{\hbar}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'} \langle \mathrm{GS}|c_\sigma^\dagger(\mathbf{p}')c_\sigma(\mathbf{p})c_\sigma^\dagger(\mathbf{k}')c_\sigma(\mathbf{k})|\mathrm{GS}\rangle. \qquad (265)$$

The expectation value $\langle \mathrm{GS}|c_\sigma^\dagger(\mathbf{p}')c_\sigma(\mathbf{p})c_\sigma^\dagger(\mathbf{k}')c_\sigma(\mathbf{k})|\mathrm{GS}\rangle$ 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. 8).

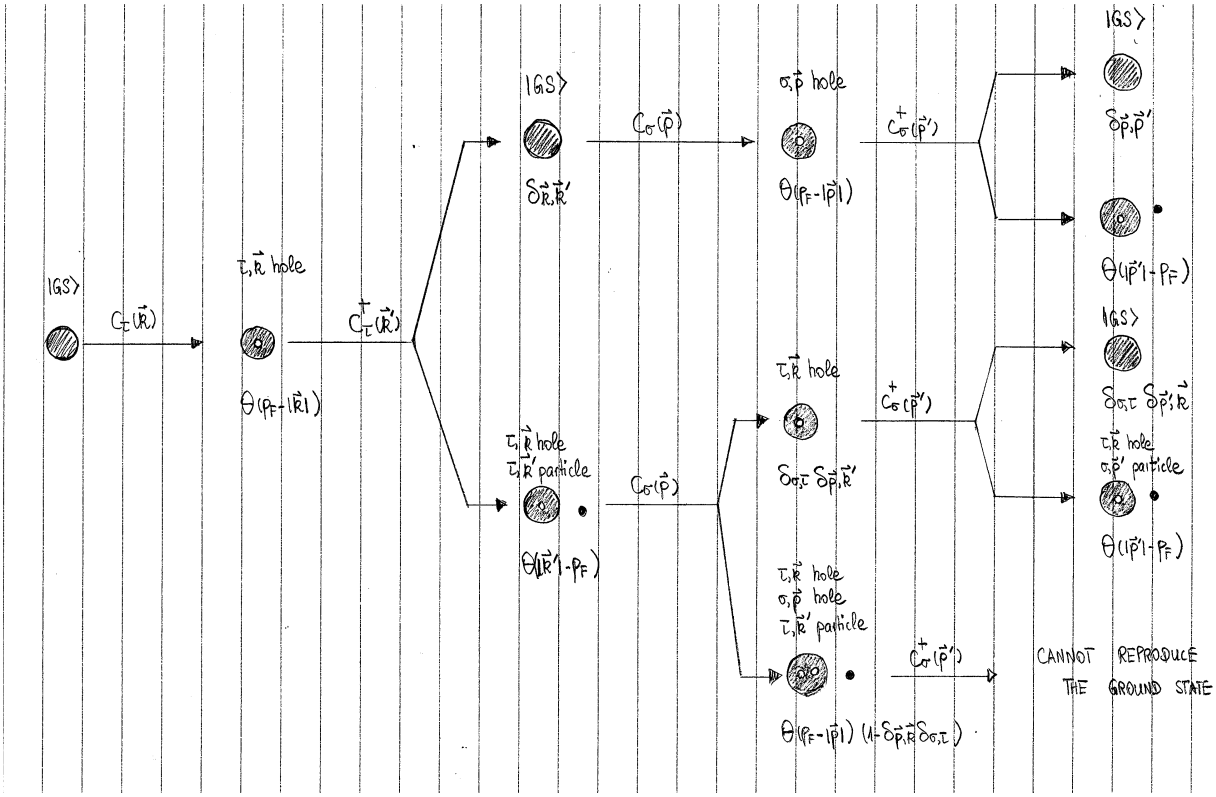


Figure 8:

The result is

$$\begin{aligned}\langle \mathrm{GS}|c_\sigma^\dagger(\mathbf{p}')c_\sigma(\mathbf{p})c_\sigma^\dagger(\mathbf{k}')c_\sigma(\mathbf{k})|\mathrm{GS}\rangle &= \delta_{\mathbf{k},\mathbf{k}'}\delta_{\mathbf{p},\mathbf{p}'}\theta(p_F-|\mathbf{p}|)\theta(p_F-|\mathbf{k}|) \\ &\quad +\delta_{\sigma,\tau}\delta_{\mathbf{p},\mathbf{k}'}\delta_{\mathbf{k},\mathbf{p}'}\theta(|\mathbf{k}'|-p_F)\theta(p_F-|\mathbf{k}|). \qquad (266)\end{aligned}$$

Substituting this back in to (265) gives

$$\begin{aligned}\langle \mathrm{GS}|\rho(\mathbf{r})\rho(\mathbf{r}')|\mathrm{GS}\rangle &= \sum_{\sigma,\sigma'} \frac{1}{L^6} \sum_{\mathbf{k},\mathbf{p}} \theta(p_F-|\mathbf{k}|)\theta(p_F-|\mathbf{p}|) \\ &+ \sum_{\sigma} \frac{1}{L^6} \sum_{\mathbf{k},\mathbf{k}'} \theta(|\mathbf{k}|-p_F)\theta(p_F-|\mathbf{k}'|) e^{\frac{i}{\hbar}(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}-\mathbf{r}')} \\ &= \langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle\langle \mathrm{GS}|\rho(\mathbf{r}')|\mathrm{GS}\rangle + 2\frac{1}{L^3} \sum_{|\mathbf{k}|>p_F} e^{\frac{i}{\hbar}\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \frac{1}{L^3} \sum_{|\mathbf{k}'|<p_F} e^{-\frac{i}{\hbar}\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')}. \qquad (267)\end{aligned}$$

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

$$\frac{1}{L^3}\sum_{|\mathbf{k}|<p_F} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} \longrightarrow \int \frac{d^3\mathbf{k}}{(2\pi\hbar)^3}\theta(p_F-|\mathbf{k}|)e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} = \int_0^\infty dp p^2 \int_0^\pi d\vartheta \sin\vartheta \int_0^{2\pi} d\varphi \, \frac{\theta(p_F-\hbar p)}{(2\pi)^3} e^{ip|\mathbf{R}|\cos\vartheta}$$
$$= \int_0^{p_F/\hbar} \frac{dp}{(2\pi)^2} p^2 \frac{2\sin(p|\mathbf{R}|)}{p|\mathbf{R}|}. \tag{268}$$

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

$$\begin{aligned} k_x &= \hbar p \sin\vartheta\cos\varphi \ , \\ k_y &= \hbar p \sin\vartheta\sin\varphi \ , \\ k_z &= \hbar p\cos\vartheta. \end{aligned} \tag{269}$$

The other sum works similarly

$$\frac{1}{L^3}\sum_{|\mathbf{k}|>p_F} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} = \frac{1}{L^3}\sum_{\mathbf{k}} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} - \frac{1}{L^3}\sum_{|\mathbf{k}|<p_F} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}}. \tag{270}$$

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

$$\frac{1}{L^3}\sum_{\mathbf{k}} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} = \delta^{(3)}(\mathbf{R}). \tag{271}$$

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

$$\int d^3\mathbf{R}\frac{1}{L^3}\sum_{\mathbf{k}} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} f(\mathbf{R}) = \frac{1}{L^3}\sum_{\mathbf{k}}\int d^3\mathbf{R} e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{R}} f(\mathbf{R}) = \frac{1}{L^3}\sum_{\mathbf{k}} \tilde{f}_{\mathbf{k}} = f(\mathbf{0}). \tag{272}$$

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

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

$$\boxed{\langle \mathrm{GS}|\rho(\mathbf{r})\rho(\mathbf{r}')|\mathrm{GS}\rangle = \langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle^2 + \langle \mathrm{GS}|\rho(\mathbf{r})|\mathrm{GS}\rangle\delta^{(3)}(\mathbf{r}-\mathbf{r}') - 2\left[\int_0^{p_F/\hbar}\frac{dp}{(2\pi)^2}p^2\frac{2\sin(p|\mathbf{r}-\mathbf{r}'|)}{p|\mathbf{r}-\mathbf{r}'|}\right]^2}. \tag{273}$$

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").

6 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

$$\hat{T} = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} c^\dagger(\mathbf{p})c(\mathbf{p}). \tag{274}$$

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

$$\hat{V} = \frac{1}{2}\int d^3\mathbf{r}d^3\mathbf{r}'\ c^\dagger(\mathbf{r})c^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')c(\mathbf{r}')c(\mathbf{r}) \tag{275}$$

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

$$V(\mathbf{r},\mathbf{r}') = U\delta^{(3)}(\mathbf{r}-\mathbf{r}'), \tag{276}$$

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

$$c(\mathbf{r}) = \frac{1}{L^{3/2}}\sum_{\mathbf{p}} e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}c(\mathbf{p}), \tag{277}$$

we have

$$\hat{V} = \frac{U}{2L^3}\sum_{\mathbf{p_1},\mathbf{p_2},\mathbf{p_3}} c^\dagger(\mathbf{p_1})c^\dagger(\mathbf{p_2})c(\mathbf{p_3})c(\mathbf{p_1}+\mathbf{p_2}-\mathbf{p_3}). \tag{278}$$

6.1 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

$$|\mathrm{GS}\rangle_0 = \frac{1}{\sqrt{N!}}\Big(c^\dagger(\mathbf{p}=\mathbf{0})\Big)^N|0\rangle. \tag{279}$$

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

$${}_0\langle\mathrm{GS}|c^\dagger(\mathbf{p}=\mathbf{0})c(\mathbf{p}=\mathbf{0})|\mathrm{GS}\rangle_0 = N. \tag{280}$$

6.2 Bogoliubov Approximation

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

$$\langle\mathrm{GS}|c^\dagger(\mathbf{p}=\mathbf{0})c(\mathbf{p}=\mathbf{0})|\mathrm{GS}\rangle = N_0 \gg 1. \tag{281}$$

However,

$$[c^\dagger(\mathbf{0})c(\mathbf{0}),\hat{V}] \neq 0, \tag{282}$$

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

$$\langle\Psi|c^\dagger(\mathbf{0})c(\mathbf{0})|\Psi\rangle \simeq N_0\ , \tag{283}$$

where N_0, crucially, is a very large number. The *Bogoliubov approximation* states that for such states we in fact have

$$\boxed{c^\dagger(\mathbf{0}) \simeq \sqrt{N_0}\ , \qquad c(\mathbf{0}) \simeq \sqrt{N_0}\ ,} \tag{284}$$

i.e. creation and annihilation operators are approximately diagonal. We then may expand H in inverse powers of N_0

$$\begin{aligned} H &= \sum_{\mathbf{p}}\frac{\mathbf{p}^2}{2m}c^\dagger(\mathbf{p})c(\mathbf{p}) \\ &\quad + \frac{U}{2L^3}N_0^2 + \frac{UN_0}{2L^3}\sum_{\mathbf{k}\neq\mathbf{0}} 2c^\dagger(\mathbf{k})c(\mathbf{k}) + 2c^\dagger(-\mathbf{k})c(-\mathbf{k}) + c^\dagger(\mathbf{k})c^\dagger(-\mathbf{k}) + c(-\mathbf{k})c(\mathbf{k}) \\ &\quad + \ldots \end{aligned} \tag{285}$$

Now use that

$$N_0 = c^\dagger(\mathbf{0})c(\mathbf{0}) = N - \sum_{\mathbf{p}\neq\mathbf{0}} c^\dagger(\mathbf{p})c(\mathbf{p}), \tag{286}$$

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

$$\rho = \frac{N}{L^3} = \text{density of particles.} \tag{287}$$

Then our Hamiltonian becomes

$$\boxed{H = \frac{U\rho}{2}N + \sum_{\mathbf{p}\neq\mathbf{0}} \underbrace{\left[\frac{\mathbf{p}^2}{2m} + U\rho\right]}_{\epsilon(\mathbf{p})} c^\dagger(\mathbf{p})c(\mathbf{p}) + \frac{U\rho}{2}\left[c^\dagger(\mathbf{p})c^\dagger(-\mathbf{p}) + c(-\mathbf{p})c(\mathbf{p})\right] + \dots} \tag{288}$$

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

6.3 Bogoliubov Transformation

Consider the creation/annihilation operators defined by

$$\begin{pmatrix} b(\mathbf{p}) \\ b^\dagger(-\mathbf{p}) \end{pmatrix} = \begin{pmatrix} \cosh(\theta_\mathbf{p}) & \sinh(\theta_\mathbf{p}) \\ \sinh(\theta_\mathbf{p}) & \cosh(\theta_\mathbf{p}) \end{pmatrix} \begin{pmatrix} c(\mathbf{p}) \\ c^\dagger(-\mathbf{p}). \end{pmatrix} \tag{289}$$

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

$$[b(\mathbf{p}), b(\mathbf{q})] = 0 = [b^\dagger(\mathbf{p}), b^\dagger(\mathbf{q})]\ , \qquad [b(\mathbf{p}), b^\dagger(\mathbf{q})] = \delta_{\mathbf{p},\mathbf{q}}. \tag{290}$$

In terms of the Bogoliubov bosons the Hamiltonian becomes

$$\begin{aligned} H \;=\; & \text{const} + \frac{1}{2}\sum_{\mathbf{p}\neq\mathbf{0}} \left[\left(\frac{\mathbf{p}^2}{2m} + U\rho\right)\cosh(2\theta_\mathbf{p}) - U\rho\sinh(2\theta_\mathbf{p})\right]\left[b^\dagger(\mathbf{p})b(\mathbf{p}) + b^\dagger(-\mathbf{p})b(-\mathbf{p})\right] \\ & - \left[\left(\frac{\mathbf{p}^2}{2m} + U\rho\right)\sinh(2\theta_\mathbf{p}) - U\rho\cosh(2\theta_\mathbf{p})\right]\left[b^\dagger(\mathbf{p})b^\dagger(-\mathbf{p}) + b(-\mathbf{p})b(\mathbf{p})\right] + \dots \end{aligned} \tag{291}$$

Now we choose

$$\tanh(2\theta_\mathbf{p}) = \frac{U\rho}{\frac{\mathbf{p}^2}{2m} + U\rho}, \tag{292}$$

as this removes the $b^\dagger b^\dagger + bb$ terms, and leaves us with a *diagonal* Hamiltonian

$$\boxed{H = \text{const} + \sum_{\mathbf{p}\neq\mathbf{0}} E(\mathbf{p})b^\dagger(\mathbf{p})b(\mathbf{p}) + \dots} \tag{293}$$

where

$$E(\mathbf{p}) = \sqrt{\left(\frac{\mathbf{p}^2}{2m} + U\rho\right)^2 - (U\rho)^2}\ . \tag{294}$$

We note that

$$E(\mathbf{p}) \longrightarrow \frac{\mathbf{p}^2}{2m} \qquad \text{for } |\mathbf{p}| \to \infty, \tag{295}$$

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

$$E(\mathbf{p}) \longrightarrow \sqrt{\frac{U\rho}{m}}|\mathbf{p}| \qquad \text{for } |\mathbf{p}| \to 0. \tag{296}$$

So here we have a *linear* dispersion.

6.4 Ground State and Low-lying Excitations

We note that the Hamiltonian (293) involves only creation/annihilation operators with $\mathbf{p} \neq 0$. Formally, the Bogoliubov transformation (289) tells us that

$$b(\mathbf{0}) = c(\mathbf{0}) \ , \tag{297}$$

because $\theta_{\mathbf{p}=\mathbf{0}} = 0$. Let us now define the vacuum state $|\tilde{0}\rangle$ by

$$b(\mathbf{p})|\tilde{0}\rangle = 0 \ . \tag{298}$$

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, our basic assumption was that

$$b(\mathbf{0})|\mathrm{GS}\rangle \simeq \sqrt{N_0}|\mathrm{GS}\rangle \ , \quad b^\dagger(\mathbf{0})|\mathrm{GS}\rangle \simeq \sqrt{N_0}|\mathrm{GS}\rangle. \tag{299}$$

In practice that is all we need to know, as it allows us to calculate correlation functions etc. However, in order to get an idea what the ground state really looks like, let us express it in the form

$$|\mathrm{GS}\rangle = \sum_{n=0}^{\infty} \frac{\alpha_n}{\sqrt{n!}} \big(b^\dagger(\mathbf{0})\big)^n |\tilde{0}\rangle \ , \tag{300}$$

where the normalization condition imposes $\sum_{n=0}^{\infty} |\alpha_n|^2 = 1$. The approximate relations (299) then imply that

$$\sqrt{n}\alpha_n \simeq \sqrt{N_0}\alpha_{n-1} \ , \quad \alpha_n \simeq \sqrt{\frac{N_0}{n+1}}\alpha_{n+1} \ , \tag{301}$$

which tell us that $\alpha_n \approx 0$ unless $n \approx N_0$. So in the zero-momentum sector we obtain an (approximately) equal-amplitude linear superposition of eigenstates with approximately N_0 $\mathbf{p} = 0$ bosons.

Low-lying excited states can now be obtained by creating Bogoliubov quasipartices, e.g.

$$b^\dagger(\mathbf{q})|\mathrm{GS}\rangle, \tag{302}$$

is a particle-excitation with energy $E(\mathbf{q}) > 0$.

6.5 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

$$N_0 = N - \sum_{\mathbf{p}\neq\mathbf{0}} c^\dagger(\mathbf{p})c(\mathbf{p}). \tag{303}$$

Thus in the ground state

$$\frac{N_0}{N} = 1 - \frac{1}{N}\sum_{\mathbf{p}\neq\mathbf{0}} \langle\tilde{0}|c^\dagger(\mathbf{p})c(\mathbf{p})|\tilde{0}\rangle. \tag{304}$$

Inverting the Bogoliubov transformation we have

$$c(\mathbf{p})|\tilde{0}\rangle = \Big[\cosh(\theta_{\mathbf{p}})b(\mathbf{p}) - \sinh(\theta_{\mathbf{p}})b^\dagger(-\mathbf{p})\Big]\,|\tilde{0}\rangle = -\sinh(\theta_{\mathbf{p}})b^\dagger(-\mathbf{p})|\tilde{0}\rangle. \tag{305}$$

Using this and its hermitian conjugate equations we find

$$\begin{aligned}
\frac{N_0}{N} &= 1 - \frac{1}{N}\sum_{\mathbf{p}\neq\mathbf{0}} \sinh^2(\theta_{\mathbf{p}}) = 1 - \frac{1}{2N}\sum_{\mathbf{p}\neq\mathbf{0}} \left[\frac{1}{\sqrt{1-\tanh^2(2\theta_{\mathbf{p}})}} - 1\right] = 1 - \frac{1}{2N}\sum_{\mathbf{p}\neq\mathbf{0}} \left[\frac{\epsilon(\mathbf{p})}{E(\mathbf{p})} - 1\right] \\
&= 1 - \frac{1}{2N}\sum_{\mathbf{p}\neq\mathbf{0}} \left[\frac{1}{\sqrt{1-\left[\frac{U\rho}{\epsilon(\mathbf{p})}\right]^2}} - 1\right].
\end{aligned} \tag{306}$$

We again turn this into an integral and evaluate it in spherical polar coordinates, which gives

$$\frac{N_0}{N} \approx 1 - \frac{\pi}{\rho}\int_0^\infty \frac{dp}{(2\pi\hbar)^3} p^2 \frac{(U\rho)^2}{\left(\frac{p^2}{2m} + U\rho\right)^2}. \tag{307}$$

The integral is proportional to $U^{3/2}$ and thus indeed small for small U.

7 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

$$S^\alpha_{\mathbf{r}} \ , \quad \alpha = x, y, z \ , \tag{308}$$

which fulfil the angular momentum commutation relations

$$[S^\alpha_{\mathbf{r}}, S^\beta_{\mathbf{r}'}] = \delta_{\mathbf{r},\mathbf{r}'} i\epsilon_{\alpha\beta\gamma} S^\gamma_{\mathbf{r}}. \tag{309}$$

We will assume that the spin are large in the sense that

$$\mathbf{S}^2_{\mathbf{r}} = \sum_\alpha \left(S^\alpha_{\mathbf{r}}\right)^2 = s(s+1) \gg 1. \tag{310}$$

An appropriate Hamiltonian for such systems was derived by Heisenberg

$$\boxed{H = -J \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'}.} \tag{311}$$

Here $\langle \mathbf{r}, \mathbf{r}'\rangle$ denote nearest-neighbour pairs of spins and we will assume that $J > 0$. The model (311) is known as the ferromagnetic *Heisenberg model*. Let us begin by constructing a basis of states. At each site we have $2s+1$ states

$$|s-n\rangle_{\mathbf{r}} = \frac{1}{\mathcal{N}} (S^-_{\mathbf{r}})^n |\uparrow\rangle_{\mathbf{r}} \ , \quad n = 0, 1, \ldots, 2s, \tag{312}$$

where $\mathcal{N}$ is a normalization constant and

$$S^z_{\mathbf{r}} |\uparrow\rangle_{\mathbf{r}} = s |\uparrow\rangle_{\mathbf{r}}, \tag{313}$$

and $S^-_{\mathbf{r}} = S^x_{\mathbf{r}} - iS^y_{\mathbf{r}}$ is the spin lowering operator on site $\mathbf{r}$. A basis of states is then given by

$$\prod_{\mathbf{r}} |s_{\mathbf{r}}\rangle_{\mathbf{r}} \ , \quad -s \le s_{\mathbf{r}} \le s \text{ spin on site } \mathbf{r}. \tag{314}$$

One ground state of H is given by

$$\boxed{|\mathrm{GS}\rangle = \prod_{\mathbf{r}} |\uparrow\rangle_{\mathbf{r}}.} \tag{315}$$

Its energy is

$$H|\mathrm{GS}\rangle = -J \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} s^2 |\mathrm{GS}\rangle = -Js^2 zN |\mathrm{GS}\rangle, \tag{316}$$

where zN is the total number of bonds in our lattice. The total spin lowering operator $S^- = \sum_{\mathbf{r}} S^-_{\mathbf{r}}$ commutes with H, i.e. $[S^-, H] = 0$, and hence

$$|\mathrm{GS}, n\rangle = \frac{1}{\mathcal{N}} \left(S^-\right)^n |\mathrm{GS}\rangle \ , \quad 0 \le n \le 2sN \tag{317}$$

are ground states as well (as they have the same energy). Here $\mathcal{N}$ is a normalization.

Proof that $|\mathrm{GS}\rangle$ is a ground state:

$$2\mathbf{S}_{\mathbf{r}}\cdot\mathbf{S}_{\mathbf{r}'}=(\mathbf{S}_{\mathbf{r}}+\mathbf{S}_{\mathbf{r}'})^2-\mathbf{S}_{\mathbf{r}}^2-\mathbf{S}_{\mathbf{r}'}^2=\mathbf{J}^2-2s(s+1). \tag{318}$$

Here $\mathbf{J}^2$ is the total angular momentum squared. Its eigenvalues follow from the theory of adding angular momenta to be

$$\mathbf{J}^2|j,m\rangle=j(j+1)|j,m\rangle\ ,\quad j=2s,2s-1,\ldots,1,0. \tag{319}$$

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

$$\begin{aligned}\langle\psi|\mathbf{J}^2|\psi\rangle &= \sum_{j,m,j',m'}\langle\psi|j,m\rangle\langle j,m|\mathbf{J}^2|j',m'\rangle\langle j',m'|\psi\rangle\\ &= \sum_{j,m}|\langle\psi|j,m\rangle|^2 j(j+1)\leq 2s(2s+1)\sum_{j,m}|\langle\psi|j,m\rangle|^2=2s(2s+1).\end{aligned} \tag{320}$$

This tells us that

$$\langle\psi|\mathbf{S}_{\mathbf{r}}\cdot\mathbf{S}_{\mathbf{r}'}|\psi\rangle\leq s^2. \tag{321}$$

This provides us with a bound on the eigenvalues of the Hamiltonian, as

$$\langle\psi|H|\psi|\rangle\geq -J_{\langle\mathbf{r},\mathbf{r}'\rangle}s^2=-Js^2Nz. \tag{322}$$

The state we have constructed saturates this bound, so must be a ground state.

Let us now consider thermal expectation values of observables $\mathcal{O}$

$$\langle\mathcal{O}\rangle_\beta=\frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}\mathcal{O}\right], \tag{323}$$

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

$$\langle\mathcal{O}\rangle_\infty=\sum_{n=0}^{2sN}\langle\mathrm{GS},\mathrm{n}|\mathcal{O}|\mathrm{GS},\mathrm{n}\rangle, \tag{324}$$

i.e. we average over all ground states. This average is independent of the choice of quantization axis, reflecting the presence of a global spin rotation symmetry. Indeed, in a rotated co-ordinate system we have

$$\langle\mathcal{O}'\rangle_\infty=\sum_{n=0}^{2sN}\langle\mathrm{GS},\mathrm{n}|e^{i\alpha\cdot\mathbf{S}}\mathcal{O}e^{-i\alpha\cdot\mathbf{S}}|\mathrm{GS},\mathrm{n}\rangle, \tag{325}$$

where $\mathbf{S}=\sum_{\mathbf{r}}\mathbf{S}_{\mathbf{r}}$ are the global spin operators. Now, $\{|\mathrm{GS},\mathrm{n}\rangle\}$ form an orthonormal basis of the subspace $\mathcal{H}_0$ of degenerate ground states of H. As $e^{-i\alpha\cdot\mathbf{S}}$ is a unitary operator *that commutes with* H, we must have

$$e^{-i\alpha\cdot\mathbf{S}}|\mathrm{GS},\mathrm{n}\rangle=\sum_{m=0}^{2sN}U_{nm}|\mathrm{GS},\mathrm{m}\rangle\ ,\quad \sum_{m=0}^{2sN}U_{nm}U^*_{ml}=\delta_{n,l}. \tag{326}$$

Substituting this back, we see that indeed $\langle\mathcal{O}'\rangle_\infty=\langle\mathcal{O}\rangle_\infty$.

In a real system, the $2sN+1$-fold ground state degeneracy is usually broken through imperfections. In particular, these will lead to *spontaneous symmetry breaking* of the spin rotational SU(2) symmetry and the emergence of a spontaneous magnetization. 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 degeneracy of the ground states, which now will have energies

$$E_{\mathrm{GS,n}} = -Js^2 zN - \epsilon s(N-2n). \tag{327}$$

Now consider the sequence of limits

$$\lim_{\epsilon\to 0}\lim_{N\to\infty}[E_{\mathrm{GS,n}} - E_{\mathrm{GS},0}] = \begin{cases} 0 & \text{if } \lim_{N\to\infty}\frac{n}{N} = 0\ , \\ \infty & \text{else.} \end{cases} \tag{328}$$

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.

We succeeded in finding the ground states of H because of their simple structure. For more general spin Hamiltonians, or even the Hamiltonian (311) with negative value of J, this will no longer work and we need a more general, but approximate way of dealing with such problems.

8 Holstein-Primakoff Transformation

Spin operators can be represented in terms of bosonic creation and annihilation operators in the form

$$S^z_{\mathbf{r}} = s - a^\dagger_{\mathbf{r}} a_{\mathbf{r}}\ , \quad S^+_{\mathbf{r}} = S^x_{\mathbf{r}} + iS^y_{\mathbf{r}} = \sqrt{2s}\sqrt{1 - \frac{a^\dagger_{\mathbf{r}} a_{\mathbf{r}}}{2s}}\, a_{\mathbf{r}}\ . \tag{329}$$

You can check that the bosonic commutation relations

$$[a_{\mathbf{r}}, a^\dagger_{\mathbf{r}'}] = \delta_{\mathbf{r},\mathbf{r}'} \tag{330}$$

imply that

$$[S^\alpha_{\mathbf{r}}, S^\beta_{\mathbf{r}'}] = \delta_{\mathbf{r},\mathbf{r}'} i\epsilon_{\alpha\beta\gamma} S^\gamma_{\mathbf{r}}. \tag{331}$$

However, there is a caveat: the spaces of QM states are different! At site $\mathbf{r}$ we have

$$\big(S_{\mathbf{r}}\big)^n |\uparrow\rangle_{\mathbf{r}}\ , \quad n = 0, \ldots, 2s \tag{332}$$

for spins, but for bosons there are infinitely many states

$$\big(a^\dagger_{\mathbf{r}}\big)^n |0\rangle_{\mathbf{r}}\ , \quad n = 0, \ldots, \infty. \tag{333}$$

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

$$\langle \mathrm{GS}|S^z_{\mathbf{r}}|\mathrm{GS}\rangle = s = \langle \mathrm{GS}|s - a^\dagger_{\mathbf{r}} a_{\mathbf{r}}|\mathrm{GS}\rangle. \tag{334}$$

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*

$$\boxed{H = -J\sum_{\langle \mathbf{r},\mathbf{r}'\rangle} s^2 - s\left[a^\dagger_{\mathbf{r}} a_{\mathbf{r}} + a^\dagger_{\mathbf{r}'} a_{\mathbf{r}'} - a^\dagger_{\mathbf{r}} a_{\mathbf{r}'} - a^\dagger_{\mathbf{r}'} a_{\mathbf{r}}\right] + \ldots} \tag{335}$$

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

$$a(\mathbf{k}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{r}}\ , \qquad [a(\mathbf{k}), a^\dagger(\mathbf{p})] = \delta_{\mathbf{k},\mathbf{p}}\ , \tag{336}$$

which gives

$$\boxed{H = -Js^2Nz - Js\sum_{\mathbf{q}} \epsilon(\mathbf{q}) a^\dagger(\mathbf{q}) a(\mathbf{q}) + \dots} \tag{337}$$

For a simple cubic lattice the energy is

$$\epsilon(\mathbf{q}) = 2Js\left[3 - \cos q_x - \cos q_x - \cos q_z\right]. \tag{338}$$

For small wave numbers this is quadratic

$$\epsilon(\mathbf{q}) \approx Js^2|\mathbf{q}|^2 \qquad \text{for } |\mathbf{q}| \to 0. \tag{339}$$

In the context of spontaneous symmetry breaking these gapless excitations are known as *Goldstone modes*.