Path integrals

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In the study of quantum mechanical many-body systems it is not so useful to write down the Schrödinger equation of $N \sim 10^{23}$ particles and attempt to solve it. Even if we somehow managed to obtain such a solution, the amount of detail in $\psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots \boldsymbol{x}_N)$ would too much information to make sense of.

A successful approach to quantum mechanical many-body physics is the approach through second quantization. However, this technique, although very useful, can be at times quite clumsy to work with. It is useful to have a different mathematical tool to deal with the same problem. The mathematical tool that is discussed here is the path integral approach. This technique is intimately related to the second-quantization approach and in particular both ways of describing a physical many-body system are equivalent. This means that anything that can be achieved by second quantization must also be achievable by the path integral method and the other way around. Sometimes, however, it is much easier to work out a problem one way than the other. So it is useful to know both techniques.

Before we discuss the many-body problem, we go back to the single-particle problem. The path integral is most easily understood in this setting. The path integral is closely connected to the concept of *action* from classical mechanics. We therefore begin with a review of this concept.

Review of the action concept

Consider a classical particle of mass m that lives in one dimension and is subject to a potential $V(x)$. We can describe this problem by means of a Lagrangian, which is the kinetic minus the potential energy,

$$L(x, \dot{x}) = \frac{m}{2}\dot{x}^2 - V(x).$$

A striking and beautiful result is that the particle always moves such that it minimizes the *classical action*. Let us imagine that the particle starts at position x_i at time t_i and is at position x_f at a later time t_f. The action is a number that we obtain by integrating the Lagrangian between the start and end times for the actual curve $x(t)$
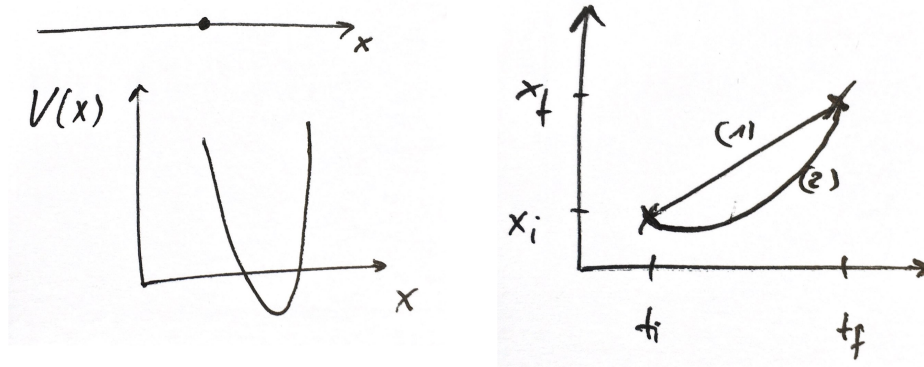
$$S = \int\limits_{t_i}^{t_f} dt \; L(x, \dot{x}).$$

Figure 1: Left: Particle moving in 1 dimension inside a potential $V(x)$ Right: paths connecting start and end points

Actually, we could plug in any curve $x(t)$ into the Lagrangian and evaluate the action. The principle of least action states that this value will be least (actually only extremal) when the true path of the particle is chosen. We can use the calculus of variations to find the curve $x(t)$ that makes the action stationary. The result is of course the equation of motion of the particle

$$\frac{\partial L(x, \dot{x})}{\partial x} - \frac{d}{dt}\frac{\partial L(x, \dot{x})}{\partial \dot{x}} = 0,$$

which tells us how the particle actually moves from x_i to x_f in the given time.

The sum over all paths

Let us now look at the same setting in the quantum context. The Hamiltonian is

$$H = \frac{P^2}{2m} + V(X),$$

where P and X are now operators and the physics of the particle is governed by the Schrödinger equation

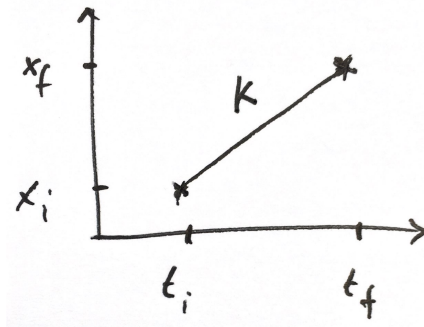$$H|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle.$$

Figure 2: Spacetime diagram of the propagator

A particle that is localized at position x_i is described quantum mechanically by the ket $|\psi\rangle = |x_i\rangle$. We can ask what is the probability amplitude to find it in the state $|x_f\rangle$ at a time $t_f - t_i$ later. We get the answer by time-evolving the state $|x_i\rangle$ and computing the overlap with $|x_f\rangle$. The answer is the probability amplitude

$$K(x_f, t_f; x_i, t_i) = \langle x_f | e^{-\frac{i}{\hbar} H \cdot (t_f - t_i)} | x_i \rangle,$$

where the object K is called the *propagator* sometimes, since it propagates a wave function $\psi(x, t_i)$ at time t_i to a wave function at time t_f:

$$\int dx' \ K(x, t_f; x', t_i)\psi(x', t_i) = \psi(x, t_f)$$

Of course, this is not a big surprise, after all $K(x_f, t_f; x_i, t_i)$ is just the time-evolution operator expressed in the x-basis. We draw a diagram for the propagator as shown in the figure. A straight edge indicates the propagator K. Of course this edge does not represent the particle's trajectory (which is not defined sharply), but rather it is to be understood as an abstract representation of the probability amplitude K.

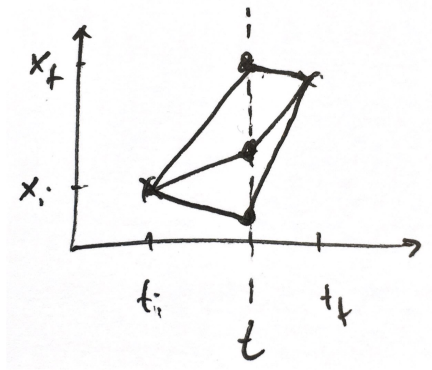There is a composition law rule for this propagator, that we look at next.

Figure 3: Composition rule for propagators

Imagine we pick a time t between t_i and t_f. Then we can write

$$K(x_f, t_f; x_i, t_i) = \langle x_f | e^{-\frac{i}{\hbar} H \cdot (t_f - t)} e^{-\frac{i}{\hbar} H \cdot (t - t_i)} | x_i \rangle$$

$$= \int dx \ \langle x_f | e^{-\frac{i}{\hbar} H \cdot (t_f - t)} | x \rangle \langle x | e^{-\frac{i}{\hbar} H \cdot (t - t_i)} | x_i \rangle$$

$$= \int dx \ K(x_f, t_f; x, t) K(x, t; x_i, t_i),$$

where in the second line we used the resolution of identity $\mathbb{1} = \int dx \ |x\rangle\langle x|$ and in the last line the result was rexpressed in terms of propagators. Let us interpret the result. The propagator for the particle to travel from x_i at t_i to x_f at t_f is the sum (integral) over the product of propagators with an intermediate point x at time t. We can show this too in a diagram.

Imagine decomposing each of the two $K's$ into two $K's$ and introducing more and more intermediate times. The result is shown in the figure. In the limit of an infinite number of intermediate points, the broken lines become a smooth curve and we end up with an integral over all curves connecting points x_i, t_i and x_f, t_f. Notice that the number of integrals, which comes from putting in resolutions of the identity, tends to infinity. This is what is called a path integral, an integral over all curves connecting given points. In the next section
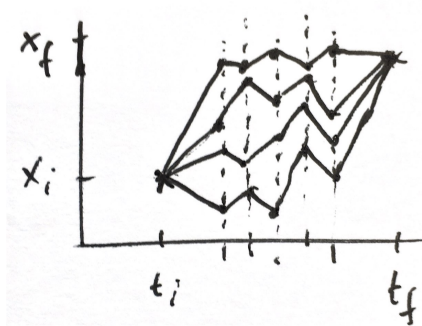
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Figure 4: One can introduce many intermediate times and integrate over the corresponding positions

we find that the propagator can be expressed as

$$K(x_f, t_f; x_i, t_i) \sim \sum_{\text{all paths } x(t)} e^{\frac{i}{\hbar} S[x(t)]},$$

where by 'all paths' we mean all paths connecting the two boundary points. In the exponential the action S has to be computed for every path that appears in the sum. Clearly this sum is a new kind of mathematical object and when we derive this result below, we will see how it has to be understood.

A nice feature of this result can be seen right away. A slight change in a path $x(t) \to x(t) + \delta x(t)$ will result in a slight change in the action $S \to S + \delta S$. If the action is large compared to $\hbar$, which is the case if the mass of the particle is macroscopic, then even for a small change δS, a large change in $\frac{i}{\hbar} S[x(t)]$ will result. As a consequence the exponential oscillates very fast and all the different paths that appear in the sum will cancel. However, for classical paths $\delta S = 0$, thus these paths will survive in the sum. In this way the classical laws (equation of motion) emerge from the quantum laws. Clearly whether a system behaves classically or quantum mechanically is governed by how the value of the action compares to $\hbar$. Treating $\hbar$ like a small parameter, we will see below that it is possible to develop a semiclassical approximation to quantum mechanics through the path integral.

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Derivation of the path integral

The composition rule for the propagator allows us to work out the propagator for an infinitesimal time $\Delta t = \frac{t_f - t_i}{N}$ and to later combine N such tiny propagators to get the full propagator. Therefore we consider

$$K(x', t + \Delta t; x, t) = \langle x'|e^{-\frac{i}{\hbar}H \cdot \Delta t}|x\rangle$$

and expand the exponential for small Δt:

$$\langle x'|e^{-\frac{i}{\hbar}H \cdot \Delta t}|x\rangle = \langle x'|\left[1 - \frac{i}{\hbar}H \cdot \Delta t + \mathcal{O}(\Delta t)^2\right]|x\rangle = \langle x'|\left[1 - \frac{i}{\hbar}[\frac{P^2}{2m} + V(X)] \cdot \Delta t + \mathcal{O}(\Delta t)^2\right]|x\rangle.$$

Here P and X are of course operators. However, when $V(X)$ acts on the position ket to the right it will become $V(x)$ and the operator turns into a regular number. We can do the same to the kinetic energy term when we insert the resolution of identity in the momentum basis $\mathbb{1} = \int dp \, |p\rangle\langle p|$:

$$\langle x'|e^{-\frac{i}{\hbar}H \cdot \Delta t}|x\rangle = \int dp \, \langle x'|p\rangle\langle p|\left[1 - \frac{i}{\hbar}[\frac{P^2}{2m} + V(X)] \cdot \Delta t + \mathcal{O}(\Delta t)^2\right]|x\rangle$$

$$= \int dp \, \langle x'|p\rangle\langle p|x\rangle\left[1 - \frac{i}{\hbar}[\frac{p^2}{2m} + V(x)] \cdot \Delta t + \mathcal{O}(\Delta t)^2\right]$$

$$= \int dp \, \langle x'|p\rangle\langle p|x\rangle \exp\left(-\frac{i}{\hbar}[\frac{p^2}{2m} + V(x)] \cdot \Delta t\right) \qquad (1)$$

In the last line we rexponentiated, which is allowed since Δt can be made arbitrarily small. Now we use that $|p\rangle$ is a normalzied plane wave state, i.e. $\langle x|p\rangle = e^{ipx/\hbar}/\sqrt{2\pi\hbar}$. This brings the propagator into the form

$$K(x', t + \Delta t; x, t) = \int dp \, \frac{e^{ip(x'-x)/\hbar}}{2\pi\hbar} \exp\left(-\frac{i}{\hbar}[\frac{p^2}{2m} + V(x)] \cdot \Delta t\right).$$

The integral over p is Gaussian and can be carried out, we find:

$$K(x', t + \Delta t; x, t) = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \, \exp\left(-\frac{m}{2i\hbar}\frac{(x'-x)^2}{\Delta t}\right)\left[\exp\left(-\frac{i}{\hbar}[V(x)] \cdot \Delta t\right)\right.$$

$$= \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \, \exp\frac{i\Delta t}{\hbar}\left(\frac{m}{2}\frac{(x'-x)^2}{\Delta t^2} - V(x)\right).$$

This is the form of the propagator for infinitesimal times Δt.

Now we can decompose the full propagator by splitting the time between t_f and t_i into N parts of size $\Delta t = (t_f - t_i)/N$:

$$K(x_f, t_f; x_i, t_i) = \int dx_{N-1} \ldots dx_1 K(x_f, t_f; x_{N-1}, t_{N-1})K(x_{N-1}, t_{N-1}; x_{N-2}, t_{N-2}) \ldots K(x_1, t_1; x_i, t_i)$$

Notice the following peculiarity. The number of integrals is $N - 1$ and we will let $N \to \infty$, i.e. we have to do an infinite number of integrations.

In the limit where N is large, Δt is small and we can express the K's on the right hand side in terms of the infinitesimal time propagator (1). Inserting the result that we found for the latter, we get:

$$K(x_f, t_f; x_i, t_i) = \int dx_{N-1} \ldots dx_1 \left[\sqrt{\frac{m}{2\pi i \hbar \Delta t}} \right]^N \exp \frac{i\Delta t}{\hbar} \sum_{i=0}^{N-1} \left(\frac{m}{2} \frac{(x_{i+1} - x_i)^2}{\Delta t^2} - V(x_i) \right),$$

where we have put

$$x_0 = x_i$$
$$t_0 = t_i$$
$$x_N = x_f$$
$$t_N = t_f.$$

Let us now look more closely at what stands inside the exponential. In the limit of $N \to \infty$, i.e. an infinite subdivision of the time interval, the sum corresponds to the definition of the Riemann integral:

$$\frac{i\Delta t}{\hbar} \sum_{i=0}^{N} \left(\frac{m}{2} \frac{(x_{i+1} - x_i)^2}{\Delta t^2} - V(x_i) \right) \to \frac{i}{\hbar} \int dt \left[\frac{m}{2} \dot{x}^2 - V(x) \right],$$

Quite amazingly we see that the action familiar to us from classical mechanics appears here.
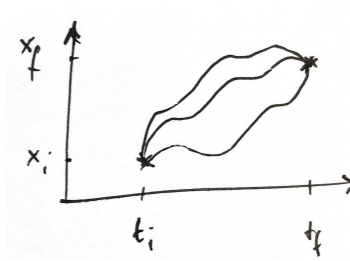

Figure 5: The zig-zag lines go over into paths as $N \to \infty$

In the limit of $N \to \infty$ the jagged, zig-zag lines become continuous curves,

see figure. We write the propagator as

$$K(x_f, t_f; x_i, t_i) = \int\limits_{\substack{x(t_i)=x_i \\ x(t_f)=x_f}} Dx(t)\; e^{\frac{i}{\hbar}S[x(t)]},$$

the differential sign under the integral stands for an infinite number of integrals:

$$\int Dx(t) = \lim_{N\to\infty} \left[\sqrt{\frac{m}{2\pi i\hbar\Delta t}}\right]^N \int dx_{N-1}\ldots dx_1$$

The mathematician would not be very happy with such a definition. But the path integral has been shown to be an incredibly useful and a fully valid tool in the exploration of physical systems. The only way to get comfortable with this strange mathematical object is to practise it on many example problems and convince oneself that the answers obtained from quantum mechanics are the same as those obtained with the path integral.

0+1 and 1+1 dimensional field theories

We have managed to write the single particle problem in terms of a path integral of $x(t)$. It turns out that this is a so-called $0 + 1$ dimensional field theory. Here 0 refers to the number of spatial dimensions and 1 to the number of time dimensions. This may seem strange at first sight, since we have thought of $x(t)$ as a spatial coordinate. But this is just a question of interpretation. We may just as well imagine that we have a scalar field ϕ (like the potential for an electric field) at one single position in space and dependent on time t. Then we would describe it by the same kind of path integral $\int D\phi(t)e^{iS[\phi]/\hbar}$ with some action for the scalar field.

Similarly, imagine that we start out with a path integral of N particles, described by coordinates $x_i(t)$ with $i = 1\ldots N$. Then in the limit $N \to \infty$ we can also interprete this path integral as a $1 + 1$ dimensional field theory. We just have to introduce a scalar field ϕ that is defined on a line with coordinates $x = ia$, where a is a lattice size. Then the field ϕ depends on two dimensions x and t: $\phi(x, t)$.

Connection of the path integral to statistical physics

One of the central themes of condensed matter physics are the equilibrium properties of many-body systems. The subject that deals with these questions is statistical physics. In statistical physics the central object is the partition function, denoted by Z. If we know the Z for a physical system, we know all of its equilibrium properties. In the statistical physics of quantum systems we start with a Hamiltonian, as for example our simple

$$H = \frac{P^2}{2m} + V(X)$$

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and we find Z by computing a trace:

$$Z = \text{Tr}[e^{-\beta H}] = \sum_n \langle n|e^{-\beta H}|n\rangle,$$

here the sum has to be extended over a complete set of states, say the energy eigenstates of H. Now we ask: how is this sum connected to path integrals? Instead of using energy eigenstates $|n\rangle$, let us switch to position eigenstates, by using $\mathbb{1} = \int dx |x\rangle\langle x|$:

$$Z = \int dx \sum_n \langle n|x\rangle\langle x|e^{-\beta H}|n\rangle = \int dx \sum_n \langle x|e^{-\beta H}|n\rangle\langle n|x\rangle = \int dx \langle x|e^{-\beta H}|x\rangle$$

This looks familiar, in fact the summand is reminiscent of a probability amplitude, except that instead of $-iH \cdot (t_f - t_i)/\hbar$ in the exponent, we have $-\beta H$ and also $x_f = x_i = x$. Let us take our result

$$\langle x_0|e^{-iHT/\hbar}|x_0\rangle = \int_{\substack{x(0)=x_0 \\ x(T)=x_0}} Dx(t)\, e^{\frac{i}{\hbar}\int_0^T dt\left[\frac{m}{2}\dot{x}^2 - V(x)\right]},$$

where $t_i = 0, t_f = T$ and make the substitutions

$$T = -i\beta\hbar$$
$$t = -i\tau$$

then we get

$$\langle x_0|e^{-\beta H}|x_0\rangle = \int_{\substack{x(0)=x_0 \\ x(T)=x_0}} Dx(t)\, e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\left[\frac{m}{2}\dot{x}^2 + V(x)\right]}.$$

Surprisingly the i in going from t to τ has changed the sign of the kinetic energy, such that in the exponent we have now the Hamiltonian and not the Lagrangian. Finally, in order to obtain the partition function we integrate over x_0. This changes the path integration such that in the boundary conditions x_0 can be anything, as long as $x(t)$ is periodic:

$$Z = \int_{x(0)=x(T)} Dx(t)\, e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\left[\frac{m}{2}\dot{x}^2 + V(x)\right]}$$

The free particle

So far we have derived path integrals, but we haven't evaluated any of them. Let us evaluate the easiest, non-trivial path integral we can think of. We get
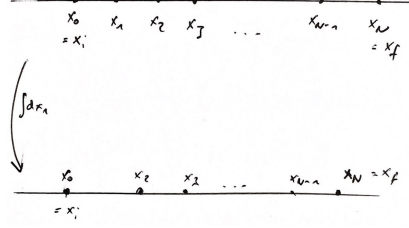
Figure 6: A variable x_i (except for x_0 ind x_N) is connected to its two neighbors x_{i-1} and x_{i+1}. After integrating over x_i, x_{i-1} and x_{i+1} become connected.

this by putting $V(x) = 0$, i.e. we want to calculate the free particle propagator

$$
K(x_f, T, x_i, 0) = \int\limits_{\substack{x(0)=x_i \\ x(T)=x_f}} Dx(t) e^{\frac{i}{\hbar}\int_0^T dt \frac{m}{2}\dot{x}^2}.
$$

It is useful to go back to the discretized definition of the path integral

$$
K(x_f, T, x_i, 0) = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2} \int dx_1 \cdots \int dx_N \exp(\frac{im}{2\hbar\Delta t}\sum_{i=0}^{N-1}(x_{i+1}-x_i)^2),
$$

where just as before we have as endpoints $x_0 = x_i$, $x_N = x_f$ and $\Delta t = T/N$. This is a somewhat tricky integral, in that each integration involves two Gaussian factors, e.g. the integral over x_1 involves $\exp(\frac{im}{2\hbar\Delta t}(x_1 - x_0)^2) \times \exp(\frac{im}{2\hbar\Delta t}(x_2 - x_1)^2)$. A neat way of doing this can be found in the excellent book of Feynman and Hibbs. This way is based on the integral identity

$$
\int\limits_{-\infty}^{\infty} dx e^{-a(x-x')^2-b(x''-x)^2} = \sqrt{\frac{\pi}{a+b}} \exp\left(-\frac{(x'-x'')^2}{\frac{1}{a}+\frac{1}{b}}\right).
$$

Let us begin by taking up first the x_1 integration:

$$
\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{2/2} \int dx_1 \exp(\frac{im}{2\hbar\Delta t}(x_1 - x_0)^2) \times \exp(\frac{im}{2\hbar\Delta t}(x_2 - x_1)^2)
$$

Here we used up two factors of $\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2}$ from the definition. The result of integrating over x_1 is

$$
\left(\frac{m}{2\pi i\hbar\ 2\Delta t}\right)^{1/2} \exp(\frac{im}{2\hbar\ 2\Delta t}(x_2 - x_0)^2).
$$

This looks just like one of the factors we started with, except that everywhere Δt has now been replaced with $2\Delta t$. Also x_1 has been removed from the sequence shown in the figure and x_2 is now linked directly to x_0.

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We continue with the integrations. Next up is the integral over the Gaussians involving x_2. We also take one factor of $\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2}$ from the definition:

$$\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2}\left(\frac{m}{2\pi i\hbar\, 2\Delta t}\right)^{1/2}\exp(\frac{im}{2\hbar\, 2\Delta t}(x_2-x_0)^2)\times\exp(\frac{im}{2\hbar\,\Delta t}(x_2-x_3)^2)$$

The result of this is:

$$\left(\frac{m}{2\pi i\hbar\, 3\Delta t}\right)^{1/2}\exp(\frac{im}{2\hbar\, 3\Delta t}(x_3-x_0)^2)$$

In the place of Δt we find $3\Delta t$ and the Gaussian connects x_3 to x_0.

Since we are already seeing the rule behind these integrations, we can now proceed recursively. After carrying out the last integration, the one over x_{N-1}, we are left with

$$K(x_f,T,x_i,0)=\left(\frac{m}{2\pi i\hbar\, N\Delta t}\right)^{1/2}\exp(\frac{im}{2\hbar\, N\Delta t}(x_N-x_0)^2)=\left(\frac{m}{2\pi i\hbar\, T}\right)^{1/2}\exp(\frac{im}{2\hbar\, T}(x_f-x_i)^2).$$

This is the final answer for the propagator. This is indeed the familiar result from doing ordinary quantum mechanics and is a good check that the path integral formalism does indeed work as expected and that furthermore the strange looking factors $\lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2}$ are in fact needed.

Gaussian integrals and Wick's theorem

In working with path integrals the most important class of Lagrangians are quadratic ones, since the corresponding path integrals can be computed exactly. The underlying reason for this is that such path integrals are Gaussian. By starting with the simplest Gaussian integral and successively generalizing we end up with Gaussian path integrals.

Let us begin with the simplest Gaussian integral

$$\int\limits_{-\infty}^{+\infty}dx\; e^{-\frac{1}{2}ax^2}=\sqrt{\frac{2\pi}{a}}$$

which is a result that holds whenever Re $a>0$. A slightly more difficult one is, if there is also a linear term in the exponent:

$$Z[J]=\int\limits_{-\infty}^{+\infty}dx\; e^{-\frac{1}{2}ax^2+Jx}$$

We can relate it to the previous version by completing the square:

$$Z[J]=\int\limits_{-\infty}^{+\infty}dx\; e^{-\frac{1}{2}a(x-J/a)^2}e^{\frac{J^2}{2a}}=\sqrt{\frac{2\pi}{a}}e^{\frac{1}{2}Ja^{-1}J}\tag{2}$$

The reason why we write the exponent in the result in this strange way, will become clearer now. Let us define averages by:

$$\langle \ldots \rangle = \left. \frac{\int\limits_{-\infty}^{+\infty} dx \ (\ldots) \, e^{-\frac{1}{2}ax^2 + Jx}}{Z[J]} \right|_{J \to 0} \tag{3}$$

The denominator is just there to normalize and we can calculate it rightaway:

$$\int\limits_{-\infty}^{+\infty} dx \ e^{-\frac{1}{2}ax^2 + Jx} \bigg|_{J \to 0} = \sqrt{\frac{2\pi}{a}}.$$

The numerator is somewhat trickier. As an example, let us calculate $\langle x^2 \rangle$. We need to find

$$\int\limits_{-\infty}^{+\infty} dx \ x^2 e^{-\frac{1}{2}ax^2 + Jx}.$$

This can be done in many ways, but a particularly elegant way is to use derivatives with respect to J:

$$\int\limits_{-\infty}^{+\infty} dx \ x^2 e^{-\frac{1}{2}ax^2 + Jx} \bigg|_{J \to 0} = \partial_J^2 \int\limits_{-\infty}^{+\infty} dx \ e^{-\frac{1}{2}ax^2 + Jx} \bigg|_{J \to 0} = \sqrt{\frac{2\pi}{a}} \partial_J^2 e^{\frac{1}{2}Ja^{-1}J} \bigg|_{J \to 0}$$

The square root factor is not important, since it will eventually be cancelled by the denominator in (3). In $\partial_J^2 e^{\frac{1}{2}Ja^{-1}J} \bigg|_{J \to 0}$ it is useful to note that we set $J = 0$ after taking the derivative, thus terms with factors of J will vanish in the end. One differentiation brings down a J and the next differentiation has to annihilate it, or else it won't make a contribution. There are two ways to bring down a J for the first ∂_J, since there are two J's in $e^{\frac{1}{2}Ja^{-1}J}$. This cancels the factor of $1/2$. In the end we are left with the simple result:

$$\langle x^2 \rangle = a^{-1}$$

Let us try to do the same for $\langle x^4 \rangle$. This gives

$$\langle x^4 \rangle = \partial_J^4 e^{\frac{1}{2}Ja^{-1}J} \bigg|_{J \to 0}.$$

Again, each ∂_J acting on the exponential brings down a J and since we are taking the $J \to 0$ limit, this will only work if two ∂_J bring down J's and two ∂_J annihilate them. Which of the ∂_J annihilates which J does not matter, as long as there is one ∂_J that generates a J and there is another ∂_J to annihilate it. There is schematic way to count in how many ways this can be done. We write $\langle xxxx \rangle$ and pair up two x's as illustrated in the figure. This corresponds to saying which ∂_J generates a J and which ∂_J annihilates it. We see from the figure that there are 3 distinct ways. In general if one has $\langle x^{2m} \rangle$ there are $\frac{(2m)!}{2^m m!} = (2m-1) \cdot (2m-3) \cdot \cdots \cdot 1$ ways. Thus the general result is

$$\langle x^{2m} \rangle = (2m-1) \cdot (2m-3) \cdot \cdots \cdot 1 \left(a^{-1} \right)^m.$$

Figure 7: Three distinct ways to pair up each of the four x's

Notice what we did: By introducing the term Jx into the exponential of the Gaussian, we found an elegant way to compute expectation values by taking derivatives of $Z[J]$. The variable J is called the source and by differentiating with respect to it, we can compute averages of powers of x.

Let us now generalize this integral to a slightly more difficult one, where we now integrate over $x_1, \ldots, x_N$:

$$\int_{-\infty}^{+\infty} dx_1 \ldots dx_N \ e^{-\frac{1}{2}\vec{x}^T A \vec{x}} = \int_{-\infty}^{+\infty} dx_1 \ldots dx_N \ e^{-\frac{1}{2}x_i A_{ij} x_j} \tag{4}$$

Here A is a matrix and in the second equality we have written the exponent out using index notation. We use the summation convention, i.e. we sum over repeated indices. We can assume without loss of generality that A is symmetric. The reason is that we are summing over x_i and x_j, which would eliminate the antisymmetric part of A anyway.

But if A is symmetric, we can diagonalize it using an orthogonal transformation O:

$$A = O^T D O \tag{5}$$

Here D is a diagonal matrix. Let us insert this form into the exponent in (4):

$$-\frac{1}{2}\vec{x}^T A \vec{x} = -\frac{1}{2}\vec{x}^T O^T D O \vec{x} = -\frac{1}{2}\left(O\vec{x}\right)^T D \left(O\vec{x}\right)$$

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We used that $(O\vec{x})^T = \vec{x}^T O^T$. Now we can change to new variables $\vec{y} = O\vec{x}$ in the integration. This gives us the integral

$$I = \int\limits_{-\infty}^{+\infty} dy_1 \ldots dy_N \ e^{-\frac{1}{2}\vec{y}^T D \vec{y}} = \int\limits_{-\infty}^{+\infty} dy_1 \ldots dy_N \ e^{-\frac{1}{2}\sum_i D_{ii} y_i^2}.$$

In the last step we used the fact that D is diagonal. If all $D_{ii} > 0$ we can do this integral (else we get a diverging integral). The integrals are decoupled and we can do each of them seperately:

$$I = \prod_{i=1}^{N} \sqrt{\frac{2\pi}{D_i}} = \frac{(2\pi)^{N/2}}{\sqrt{D_{11}\ldots D_{NN}}} = \frac{(2\pi)^{N/2}}{\sqrt{\det D}} = \frac{(2\pi)^{N/2}}{\sqrt{\det A}}$$

In the penultimate step we used the fact that the determinant of D is equal to product of its diagonal entries. In the last step we used the fact that a similarity transformation like (5) does not change the determinant. Finally, in going from variables x to y there would be a Jacobian, but this is 1 (here is another exercise).

In order to make this result useful for us we introduce a source term $\vec{J} \cdot \vec{x}$ into the exponent as before:

$$Z[J] = \int\limits_{-\infty}^{+\infty} dx_1 \ldots dx_N \ e^{-\frac{1}{2}\vec{x}^T A \vec{x} + \vec{J} \cdot \vec{x}}$$

We could derive this integral by going through the same steps as before, but it is just as easy to guess the result by looking at the 1D result (2):

$$Z[J] = \int\limits_{-\infty}^{+\infty} dx_1 \ldots dx_N \ e^{-\frac{1}{2}\vec{x}^T A \vec{x} + \vec{J} \cdot \vec{x}} = \frac{(2\pi)^{N/2}}{\sqrt{\det A}} e^{\frac{1}{2}\vec{J}^T A^{-1} \vec{J}} \tag{6}$$

This is our final result. We can use it to compute Gaussian averages that we define by

$$\langle \ldots \rangle = \frac{\int\limits_{-\infty}^{+\infty} dx_1 \ldots dx_N \ (\ldots) e^{-\frac{1}{2}\vec{x}^T A \vec{x} + \vec{J} \cdot \vec{x}}}{Z[J]} \Bigg|_{J \to 0}.$$

Notice once again that the denominator is just there to cancel the factor $\frac{(2\pi)^{N/2}}{\sqrt{\det A}}$ in (6). Let us begin with the average

$$\langle x_i x_j \rangle.$$

We obtain it from (6) by differentiating:

$$\langle x_i x_j \rangle = \partial_{J_i} \partial_{J_j} e^{\frac{1}{2}\vec{J}^T A^{-1} \vec{J}} \Bigg|_{J \to 0} = \left(A^{-1} \right)_{ij}$$

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$$\langle x_i x_j x_k x_\ell \rangle = (A^{-1})_{ij}(A^{-1})_{k\ell}$$

$$\langle x_i x_j x_k x_\ell \rangle = (A^{-1})_{ik}(A^{-1})_{j\ell}$$

$$\langle x_i x_j x_k x_\ell \rangle = (A^{-1})_{i\ell}(A^{-1})_{jk}$$

$$\langle x_i x_j x_k x_\ell \rangle = (A^{-1})_{ij}(A^{-1})_{k\ell} + (A^{-1})_{ik}(A^{-1})_{j\ell} + (A^{-1})_{i\ell}(A^{-1})_{jk}$$

Figure 8: Wick pairings in vector version

Again, since we are taking the $J \to 0$ limit, one operator ∂_j brings down a $\vec{J}$, the other annihilates it. Similarly we can look at

$$\langle x_i x_j x_k x_l \rangle$$

and apply four derivatives:

$$\partial_{J_i} \partial_{J_j} \partial_{J_k} \partial_{J_l} e^{\frac{1}{2} \vec{J}^T A^{-1} \vec{J}} \Big|_{J \to 0}$$

The end result is:

$$\langle x_i x_j x_k x_l \rangle = (A^{-1})_{ij}(A^{-1})_{kl} + (A^{-1})_{ik}(A^{-1})_{jl} + (A^{-1})_{il}(A^{-1})_{jk}$$

The general pattern is quite clear now. In order to compute

$$\langle x_{i_1} x_{i_2} \ldots x_{i_{2m}} \rangle$$

we just pair up (people say 'contract') the x's in all possible ways and for each pairup of index i_a with i_b we write the factor $(A^{-1})_{i_a i_b}$:

$$\langle x_{i_1} x_{i_2} \ldots x_{i_{2m}} \rangle = \sum_{\text{all pairings}} (A^{-1})_{ab} \ldots (A^{-1})_{cd}$$

This identity is called Wick's theorem and here it is shown in the special setting of Gaussian multiple integrals.

Now we can take up our final generalization to path integrals. A function $\phi(x)$ can be be discretized at certain points along the x-axis at points $x = ia$, where a is a lattice constant and $i = 0, \pm 1, \pm 2, \ldots$. Then at each one of these points in space the function takes on a value $\phi_i := \phi(x = ia)$. Thus a function can be viewed as a vector with infinitely many components ϕ_i. If we make take a progressively smaller, we obtain an ever more accurate description of the function $\phi(x)$. The continuum analogue of $\sum_i \phi_i \psi_i$ is then $\int dx\, \phi(x)\psi(x)$. Similarly, if one has a matrix A, then the continuum analogue of the expression $\sum_{ij} \phi_i A_{ij} \psi_j$ is given by $\int dx \int dy\, \phi(x) A(x, y) \psi(y)$.
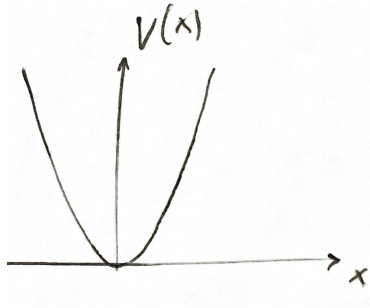
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Figure 9: Potential of a 1D particle

Then how does one define the continuum inverse of $A(x, y)$? The inverse of a matrix is defined by

$$\sum_j A_{ij}(A^{-1})_{jk} = \delta_{ik}$$

and therefore the continuum inverse of $A(x, y)$ is defined by

$$\int dy \ A(x, y)A^{-1}(y, z) = \delta(x - z).$$

Now let us look at Gaussian integral with functions instead of vectors. By analogy with the identity in equation (6), we consider

$$Z[J] = \int Dx \ \exp\left(-\frac{1}{2}\int dt \int dt' \ x(t)A(t, t')x(t') + \int dt \ J(t)x(t)\right), \quad (7)$$

where we have decided to call the field x and to use as the 'component index' the symbols t and t'. This is intentional so we can recognize this integral as a path integral. The identity (6) also suggest the result for this integral. It is:

$$Z[J] \sim \frac{1}{\sqrt{\det A}}\int Dx \ \exp\left(\frac{1}{2}\int dt \int dt' \ J(t)A^{-1}(t, t')J(t')\right) \quad (8)$$

We have dropped the constant $(2\pi)^N$, which would diverge in our case. But since we will use this formula only to compute averages , the constant will not matter. Since A is an operator here, it is not immediately clear how the determinant is computed. We shall next demonstrate on a standard example how this is done.

Semiclassical approximation

We take the problem of a particle moving in one dimension in a potential as shown in the figure. The minimum of V is at $x = 0$ and $V(x = 0) = 0$. We

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want to compute the amplitude

$$\langle 0| \exp(-iHT/\hbar)|0\rangle = \int Dx(t) \; \exp(\frac{i}{\hbar} \int\limits_0^T dt \left[\frac{m}{2}\dot{x}^2 - V(x)\right]).$$

If V is some general potential we will not be able to compute the result exactly. Thus we resort to an approximation that is know as the *semiclassical approximation.* In this approximation one assumes that the most dominant contribution to the path integral on the right hand side is the classical solution of the problem $x_{\mathrm{cl}}(t)$ plus a little bit of fluctuations $\eta(t)$:

$$x(t) = x_{\mathrm{cl}}(t) + \eta(t)$$

Inserting this into the action and expanding for small η, we obtain

$$S[x] = \int\limits_0^T dt \left[\frac{m}{2}\dot{x}_{\mathrm{cl}}^2 - V(x_{\mathrm{cl}}) + \frac{m}{2}\dot{\eta}^2 - \frac{1}{2}\frac{\partial^2 V}{\partial x^2}\eta^2\right],$$

where $\frac{\partial^2 V}{\partial x^2}$ has to be evaluated at x_{cl}. Notice that we have dropped all the linear parts in x_{cl}. The reason is that this part is exactly zero, since the classical solution has the property that $\delta S[x_{\mathrm{cl}}] = 0$.

Inside the brackets we recognize the first two terms as the classical Lagrangian, thus we write

$$S[x] = S_{\mathrm{cl}} + \int\limits_0^T dt \left[\frac{m}{2}\dot{\eta}^2 - \frac{1}{2}\frac{\partial^2 V}{\partial x^2}\eta^2\right].$$

So far everything is general and it is clear that we can always compute the resulting path integral, since the problem is quadratic in η.

We specialize now to our potential. We first have to find the classical solutions (there will in general be many) subject to the condition that the particle starts at $x = 0$ and returns to $x = 0$ at time T. There are many classical solutions that we can include, but the most important is $x_{\mathrm{cl}} = 0$. In this case the classical action is $S_{\mathrm{cl}} = 0$. Also, in order to make the action of the η part look like a harmonic oscillator, we set $\frac{\partial^2 V}{\partial x^2} = m\omega^2$. This results in the approximation for the amplitude:

$$\langle 0| \exp(-iHT/\hbar)|0\rangle = \int D\eta(t) \; \exp(\frac{i}{\hbar} \int\limits_0^T dt \left[\frac{m}{2}\dot{\eta}^2 - \frac{m\omega^2}{2}\eta^2\right]).$$

We recognize this as the path integral (7) with $J = 0$. However, we first have to bring the quadratic part into the same form, which we can do by partially integrating the first term:

$$S[x] = \frac{m}{2}\int\limits_0^T dt \left[\dot{\eta}^2 - \omega^2\eta^2\right] = -\frac{m}{2}\int\limits_0^T dt \int dt' \; \eta(t')\delta(t-t') \left[\partial_t^2 + \omega^2\right]\eta(t)$$

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To bring it completely into the same form we have also introduced an integral over t' and multiplied the integrand with a δ(t-t'), but it turns out that this only clutters up the calculation and later on, when we are more familiar with functional determinants, we will not be so careful anymore. We now read off that

$$A(t,t') = m\delta(t-t')\left[\partial_t^2 + \omega^2\right]$$

and the result for the path integral is

$$Z[J=0] \sim \frac{1}{\sqrt{\det[A]}}.$$

How do we calculate this determinant? We make use of the fact about determinants that they are equal to the product of eigenvalues. Thus we have to study the eigenvalues of A, i.e. we look for solutions of

$$m\left[\partial_t^2 + \omega^2\right]\psi = \lambda\psi. \tag{9}$$

But we have to keep in mind that there are boundary conditions to the path integral. Since $x(T) = x(0)$ we have $\eta(T) = \eta(0)$. The solutions to (9) are given by

$$\psi(t) = \sin\left(\frac{n\pi}{T}t\right)$$

with $n = 1, 2 \dots$. The eigenvalues are obtained by substituting back into the differential equation:

$$\lambda = m\left(\frac{n^2\pi^2}{T^2} - \omega^2\right).$$

The determinant is the product of these eigenvalues, thus

$$\det A = \prod_{n=1}^{\infty}\left[m\left(\frac{n^2\pi^2}{T^2} - \omega^2\right)\right].$$

This looks like a horribly divergent result. But we remember that our result (8) was left unspecified up to a constant, which was infinitely large. We can guess that this is what will cancel the divergence here. In order to find the result, we proceed as follows. There is one result for the path integral that we have worked out carefully and that we know is right. It is the result for the free problem, which gave $\langle 0|\exp(-iHT/\hbar)|0\rangle = \sqrt{\frac{m}{2\pi i\hbar T}}$. Our current problem reduces to the free problem, when we set $\omega = 0$ (this is the same as having $V = 0$ everywhere). Thus we are saying

$$\langle 0|\exp(-iHT/\hbar)|0\rangle = \frac{\langle 0|\exp(-iHT/\hbar)|0\rangle}{\langle 0|\exp(-iHT/\hbar)|0\rangle_{\text{free}}}\sqrt{\frac{m}{2\pi i\hbar T}}$$

$$= \prod_{n=1}^{\infty}\left[m\left(\frac{n^2\pi^2}{T^2} - \omega^2\right)\right]^{-1/2}\prod_{n=1}^{\infty}\left[m\left(\frac{n^2\pi^2}{T^2}\right)\right]^{1/2}\sqrt{\frac{m}{2\pi i\hbar T}}$$

$$= \prod_{n=1}^{\infty}\left[\left(1 - \frac{T^2\omega^2}{n^2\pi^2}\right)\right]^{-1/2}\sqrt{\frac{m}{2\pi i\hbar T}}$$

Now we can use a product formula that is due to L. Euler, who found it in working on the so-called Basel problem (1735):

$$\sin(x) = x \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{\pi^2 n^2} \right)$$

We thus obtain the final result:

$$\langle 0| \exp(-iHT/\hbar)|0\rangle = \left[\frac{\sin \omega T}{\omega T} \right]^{-1/2} \sqrt{\frac{m}{2\pi i \hbar T}} = \sqrt{\frac{m\omega}{2\pi i \hbar \sin \omega T}}$$

In the limit $\omega \to 0$ we see that result reduces to the free problem. In the case, where the $V(x)$ is quadratic, this is an exact result. For other V's this is of course only an approximation.

Many-body physics using the field integral

The view of quantum field theory is that each particle type has an underlying field, which can be disturbed to produce an excitation that we recognize as a particle. If we excite the electromagnetic field we produce a particle called the photon. An example from condensed matter physics, is the concept of lattice vibrations. Since the underlying stuff that is moving are the particles making up the lattice, and since those are described by quantum mechanics, the vibrations themselves are quantized. The corresponding field is called the phonon field and the excitations are called phonons. For the purposes of condensed matter physics these *quasiparticles* are just as real as elementary particles.

We have seen how quantum many-body problem can be formulated in the language of second quantization. For example, the quantum many-body problem of fermions interacting with each other is described by

$$H = \sum_{\boldsymbol{k}} \frac{\boldsymbol{k}^2}{2m} a_{\boldsymbol{k}\sigma}^+ a_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} \frac{e^2}{q^2} a_{\boldsymbol{k}-\boldsymbol{q}\sigma}^+ a_{\boldsymbol{k}'+\boldsymbol{q}\sigma'}^+ a_{\boldsymbol{k}'\sigma'} a_{\boldsymbol{k}\sigma}.$$

Our task in this section is to find a formulation of this problem in terms of something like a path integral, which is called the field integral. The difference to our previous problem is that we have here a second-quantized Hamiltonian, while before we had a conventional (sometimes called first-quantized) Hamiltonian. Recall how we handled the conventional Hamiltonian: We started with the time evolution operator $\exp(i/\hbar HT)$ that we sliced into small pieces $\exp(i/\hbar H \Delta t)$, which could be expanded in Δt. Then we inserted $|x\rangle$'s and $|p\rangle$'s at the right places that converted the operator H into an ordinary number, since these are the eigenstates of the kinetic and potential energy parts of H.

In order to construct the field integral we will have to find states that turn the second quantized operators H into ordinary numbers. We need a state that is an eigenstate of the second quantized operators. Such a state is called a *coherent state*. These coherent states turn out to be different depending on whether one

has bosons or fermions. In the case of fermions one needs to introduce a new kind of mathematical object called a Grassmann variable. We will therefore first tackle the coherent states for bosons. After we have done that, introducing Grassmann variables will be only one additional step that has to be taken in order to arrive at the fermion coherent states.

Coherent states

Let us begin with the simplest case, where our system has only one state and we can fill it up with bosons. We can populate the state by acting with a^+ and we can depopulate the state using a. Then acting with a^+'s on the vacuum of Fock space $|0\rangle$, we obtain consecutively the Fock states with more and more bosons. The state with n-particles is given by

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^+)^n|0\rangle.$$

Let $|\phi\rangle$ now be an eigenstate of a (the operator a^+ has no eigenstates). We can represent any Fock space state by a superposition of basis states $|n\rangle$, thus:

$$|\phi\rangle = \sum_n \phi_n|n\rangle \tag{10}$$

We want

$$a|\phi\rangle = \phi|\phi\rangle,$$

where ϕ is the eigenvalue associated with state $|\phi\rangle$. Acting with a on (10) we thus obtain:

$$\phi|\phi\rangle = a|\phi\rangle = \sum_n \phi_n a|n\rangle = \sum_n \phi_n \sqrt{n}|n-1\rangle = \sum_n \phi_{n+1}\sqrt{n+1}|n\rangle$$

Thus by comparing the coefficients on both sides, we obtain

$$\phi\phi_n = \phi_{n+1}\sqrt{n+1}$$

$$\rightarrow \phi_{n+1} = \frac{\phi}{\sqrt{n+1}}\phi_n.$$

We can easily solve this recursing by unfolding it step by step:

$$\phi_{n+1} = \frac{\phi}{\sqrt{n+1}}\phi_n = \frac{\phi^2}{\sqrt{n+1}\sqrt{n}}\phi_{n-1} = \cdots = \frac{\phi^{n+1}}{\sqrt{(n+1)!}}\phi_0$$

Thus we have the result that

$$|\phi\rangle = \sum_{n=0}^{\infty} \frac{\phi^n}{\sqrt{n!}}|n\rangle = \sum_{n=0}^{\infty} \frac{(\phi a^+)^n}{n!}|0\rangle = \exp(\phi a^+)|0\rangle$$

is an eigenstate of a:

$$a|\phi\rangle = \phi|\phi\rangle.$$

By taking a hermitian conjugate of this equation we obtain another identity:

$$\langle\phi|a^+ = \langle\phi|\phi^*,$$

i.e. the a^+ has a left eigenstate.

The state $|\phi\rangle$ is a superposition of Fock states with different particle numbers. This is a weird concept from the point of view of conventional N particle quantum mechanics, where the number of particles in a system never changes. But it will prove to be an extremely useful concept when dealing with second quantized Hamiltonians that allow for particle number changes.

In the derivation we will need a few identities. Let us discuss these briefly. We will need to know what is the overlap between two different states $|\phi_1\rangle$ and $|\phi_2\rangle$. To compute this we just have to apply the definitions:

$$\langle\phi_2|\phi_1\rangle = \sum_{m=0}^{\infty} \frac{\phi_2^{*m}}{\sqrt{m!}}\langle m| \sum_{n=0}^{\infty} \frac{\phi_1^n}{\sqrt{n!}}|n\rangle = \sum_{n=0}^{\infty} \frac{(\phi_1\phi_2^*)^n}{n!} = \exp(\phi_2^*\phi_1)$$

Thus we see that two coherent states are never orthogonal, they always have a finite inner product.

When we construct the field integral below, we will have to insert resolutions of identity involving coherent states. Thus we need to know how to represent $\mathbb{1}$ by something like $\int d\phi|\phi\rangle\langle\phi|$. The correct identity turns out to be

$$\mathbb{1} = \int\limits_{-\infty}^{+\infty} \int\limits_{-\infty}^{+\infty} \frac{d\phi_x d\phi_y}{\pi} \; e^{-\phi^*\phi}|\phi\rangle\langle\phi|,$$

where ϕ_x and ϕ_y are the real and imaginary part of ϕ. The integration is thus extended over all the values of ϕ in the complex plane. This completeness relation is a also the reason why ϕ has to be complex. We will now see this in the proof.

To demonstrate this identity we use the definition of $|\phi\rangle$:

$$\int\limits_{-\infty}^{+\infty} \int\limits_{-\infty}^{+\infty} \frac{d\phi_x d\phi_y}{\pi} \; e^{-\phi^*\phi}|\phi\rangle\langle\phi| = \sum_{n,m=0}^{\infty} \int\limits_{-\infty}^{+\infty} \int\limits_{-\infty}^{+\infty} \frac{d\phi_x d\phi_y}{\pi} \; e^{-\phi^*\phi} \frac{\phi^n}{\sqrt{n!}}|n\rangle\langle m|\frac{\phi^{*m}}{\sqrt{m!}}$$

In order to further evaluate it, we change from the ϕ_x, ϕ_y integration to polar coordinats: $\phi_x = \rho\cos\theta$ and $\phi_y = \rho\sin\theta$:

$$\sum_{n,m=0}^{\infty} \int\limits_{0}^{\infty} \int\limits_{0}^{2\pi} \frac{d\rho\rho d\theta}{\pi} \; e^{-\rho^2} \frac{\rho^{n+m}e^{i(n-m)\theta}}{\sqrt{n!}}|n\rangle\langle m|\frac{1}{\sqrt{m!}}$$

The integration over θ kills all terms in the double sum except for the $n=m$ terms:

$$\sum_{n=0}^{\infty} \int\limits_{0}^{\infty} \frac{d\rho\rho 2\pi}{\pi} \; e^{-\rho^2} \frac{\rho^{2n}}{n!}|n\rangle\langle n|$$

Now we take up the integration over ρ by changing to a variable $u = \rho^2$:

$$\int\limits_0^\infty d\rho\rho \; e^{-\rho^2}\rho^{2n} = \frac{1}{2}\int\limits_0^\infty du \; e^{-u}u^n = \frac{n!}{2}$$

Thus we obtain

$$\int\limits_{-\infty}^{+\infty}\int\limits_{-\infty}^{+\infty} \frac{d\phi_x d\phi_y}{\pi} \; e^{-\phi^*\phi}|\phi\rangle\langle\phi| = \sum_{n=0}^{\infty} \frac{n!}{2}\frac{2\pi}{\pi}\frac{1}{n!}|n\rangle\langle n| = \sum_{n=0}^{\infty}|n\rangle\langle n| = \mathbb{1},$$

ie.. we obtain the $\mathbb{1}$ in Fock-space. Note that it was crucial to have complex numbers as the domain of integration. If we had only allowed real ϕ's the phase factor $e^{i(n-m)\theta}$ would not have appeared and we wouldn't have produced the sum over $|n\rangle\langle n|$.

So far we have dealt with the simplest case of bosons occupying a single state created by a. In general a boson can exist in many states and we will have at least one additional quantum number specifying the state. Thus we will have operators a_i^+ with many different values of i, creating bosons in various quantum states. Since boson creation operators commute it is straightforward to generalize the coherent state construction from above to this more general setting. Only the notation gets a little bit more elaborate. The Fock-space is spanned by the occupation number basis states:

$$|n_1 n_2 \ldots\rangle$$

which describes a state occupied by n_1 bosons in state $i = 1$, n_2 bosons in state $i = 2$ and so on. It is formally constructed by acting on the Fock space vacuum with

$$|n_1 n_2 \ldots\rangle = \frac{(a_1^+)^{n_1}}{\sqrt{n_1!}} \frac{(a_2^+)^{n_2}}{\sqrt{n_2!}} \ldots |0\rangle$$

We find that the state defined by

$$|\phi\rangle = \prod_i \exp\left(\phi_i a_i^+\right)|0\rangle = \exp\left(\sum_i \phi_i a_i^+\right)|0\rangle$$

is a coherent state for all the operators a_i. The second equality holds because all the a_i^+ commute with each other. It is clear that $|\phi\rangle$ is a coherent state since a_i commutes with all a_j^+ for $j \neq i$. Thus

$$a_j|\phi\rangle = a_j \prod_i \exp\left(\phi_i a_i^+\right)|0\rangle = \phi_j \prod_i \exp\left(\phi_i a_i^+\right)|0\rangle = \phi_j|\phi\rangle$$

for all j. Thus $|\phi\rangle$ is a coherent state for all annihilation operators.

Returning with this $|\phi\rangle$ to the rules we found above, it is easy to generalize them:

$$\langle\phi'|\phi\rangle = \exp(\sum_i \phi_i^{'*}\phi_i)$$

The completeness relation becomes

$$\mathbb{1} = \int\limits_{-\infty}^{+\infty} \prod_i \int\limits_{-\infty}^{+\infty} \frac{d\phi_{ix}d\phi_{iy}}{\pi} \exp(-\sum_i \phi_i^*\phi_i)|\phi\rangle\langle\phi| = \int d(\phi^*,\phi) \ \exp(-\sum_i \phi_i^*\phi_i)|\phi\rangle\langle\phi|.$$

(11)

In the last equality we have combined all the integrations over the (infinite) product over states i into one symbol $\int d(\phi^*,\phi)$. These are all the results we need to derive the field integral for any body systems.

Field integral for many body systems

Similar to what we have learned for single particle systems, the central object in equilibrium many-body physics is the partition function Z. Once we have a handle on Z we can derive all kinds of equilibrium properties of a many-body system, as for example correlation functions that can be measured in experiments. These correlation functions are similar to the averages that we computed using Wick's theorem. After expressing the partition function as a field integral we can using all those results to compute these averages.

We begin with a second-quantized Hamiltonian. It is enough for us to take a schematic form of the type

$$H = \sum_{ij} T_{ij} a_i^+ a_j + \sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_k a_l.$$

For instance, the a's could be the annihilation operators for momentum eigenstates. Then the first term would be a kinetic energy and the second term would provide interactions between the particles. The gandcanonical partition function is given by

$$Z = \mathrm{Tr}e^{-\beta(H-\mu N)} = \sum_n \langle n|e^{-\beta(H-\mu N)}|n\rangle,$$

where n are all the Fock space states. The operator N is the particle number operator that counts the number of particles in the system and is given by

$$N = \sum_i a_i^+ a_i.$$

The parameter μ is the chemical potential that we can adjust to set the number of particles to the desired value.

As with the single particle problem we perform a change of basis from the states $|n\rangle$ to the coherent states that we have been developing. We do this by inserting the resolution of identity (11):

$$Z = \int d(\phi^*,\phi) \ e^{-\sum_i \phi_i^*\phi_i} \cdot \sum_n \langle n|\phi\rangle\langle\phi|e^{-\beta(H-\mu N)}|n\rangle$$

Now we move $\langle n|\phi\rangle$ to the very right and use $\sum_n |n\rangle\langle n| = 1$ to bring Z into the form:

$$Z = \int d(\phi^*, \phi) \; e^{-\sum_i \phi_i^* \phi_i} \cdot \langle\phi|e^{-\beta(H-\mu N)}|\phi\rangle$$

Notice that $\hbar\beta$ has units of time. In fact the exponential looks like a time evolution operator with *imaginary time*. We therefore proceed as we did with the path integral. We slice the exponential into M factors by dividing the imaginary time $\hbar\beta$ into M parts (we use the symbol M in order to distinguish it from the particle operator N):

$$Z = \int d(\phi^*, \phi) \; e^{-\sum_i \phi_i^* \phi_i} \cdot \langle\phi|e^{-\frac{\beta\hbar}{M}\frac{1}{\hbar}(H-\mu N)} \cdots e^{-\frac{\beta\hbar}{M}\frac{1}{\hbar}(H-\mu N)}|\phi\rangle$$

Now we insert the identity (11) between the exponentials. This adds $M-1$ integrations. We label the integrals by $\int d(\phi^{(n)*}, \phi^{(n)})$. Let us look at what happens to an exponential factor when we do this. We will have factors that look like this

$$\langle\phi^{(n+1)}|e^{-\frac{\beta\hbar}{M}\frac{1}{\hbar}(H-\mu N)}|\phi^{(n)}\rangle$$

Now in the limit where M is very large (in the end we let $M \to \infty$), the exponent can be expanded to first order. After that we can let the coherent states $|\phi^{(n)}\rangle$ and $\langle\phi^{(n+1)}|$ act on the Hamiltonian and N operator and re-exponentiate everything. The effect of this is to replace the a^+ and a operators by $\phi^{(n+1)*}$ and $\phi^{(n)}$ respectively. We denote this Hamiltonian by $H(\phi^{(n+1)*}, \phi^{(n)})$ and the N operator by $N(\phi^{(n+1)*}, \phi^{(n)})$. Thus we obtain

$$\langle\phi^{(n+1)}|e^{-\frac{\beta}{M}(H-\mu N)}|\phi^{(n)}\rangle = e^{-\frac{\beta\hbar}{M}\frac{1}{\hbar}(H(\phi^{(n+1)*},\phi^n)-\mu N(\phi^{(n+1)*},\phi^n))}\langle\phi^{(n+1)}|\phi^{(n)}\rangle$$

$$= e^{-\frac{\beta\hbar}{M}\frac{1}{\hbar}(H(\phi^{(n+1)*},\phi^n)-\mu N(\phi^{(n+1)*},\phi^n))}e^{\sum_i \phi_i^{(n+1)*}\phi_i^{(n)}}$$

Where we have used the overlap formula to compute $\langle\phi^{(n+1)}|\phi^{(n)}\rangle$. You see that these formulas become somewhat unwieldy, since we are also carrying around a sum over the index i. Let us suppress this sum, we can always put it back later. With this the partition function becomes

$$Z = \prod_{n=1}^N \int d(\phi^{(n)*}, \phi^{(n)}) \; e^{-\sum_{n=1}^M \phi^{(n)*}\phi^{(n)}} e^{\sum_{n=0}^M \phi^{(n+1)*}\phi^{(n)} - \frac{\beta\hbar}{M}\frac{1}{\hbar}(H(\phi^{(n+1)*},\phi^n)-\mu N(\phi^{(n+1)*},\phi^n))}$$

$$= \prod_{n=1}^N \int d(\phi^{(n)*}, \phi^{(n)}) \; e^{\Delta\sum_{n=0}^{M-1}\left[\frac{\left(\phi^{(n+1)*}-\phi^{(n)}\right)}{\Delta}\phi^{(n)} - \frac{1}{\hbar}(H(\phi^{(n+1)*},\phi^n)-\mu N(\phi^{(n+1)*},\phi^n))\right]}$$

where we defined $\Delta = \frac{\beta\hbar}{M}$ and by $\phi^{(0)} = M$ we mean ϕ.

Let us now take the continuum limit $M \to$. We obtain

$$Z = \int_{\phi(0)=\phi(\beta\hbar)} D(\phi^*, \phi) e^{-\frac{1}{\hbar}S[\phi^*,\phi]} \tag{12}$$

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with

$$S[\phi^*, \phi] = \int\limits_0^{\beta\hbar} d\tau \left[\hbar\phi^*\partial_\tau\phi + H(\phi^*, \phi) - \mu N(\phi^*, \phi)\right]$$

and also we lumped the coherent state integrals into one big functional integral

$$\int D(\phi^*, \phi) = \int d(\phi^{(n)*}, \phi^{(n)}).$$

Since in our derivation we noted that $\phi^{(0)} = \phi^{(M)}$, the integral in (12) has to carried out with the restriction that $\phi(\tau = 0) = \phi(\tau = \beta\hbar)$, i.e. we perform a big functional integral over field configurations with the condition that after the imaginary time $\beta\hbar$ has passed the fields are back to the way they were.

The Field integral for fermions

There is something peculiar that goes on when we try to construct a coherent state for fermionic systems. Let the creation operators for fermions be a_i^+. We know that fermions satsify the Pauli principle and thus have an anti-commutation relation between them:

$$a_i a_j^+ + a_j^+ a_i = \delta_{ij}$$
$$aa = a^+ a^+ = 0$$

Now imagine that $|\psi\rangle$ is a coherent state for fermions, i.e.

$$a_i|\psi\rangle = \psi_i|\psi\rangle$$
$$a_j|\psi\rangle = \psi_i|\psi\rangle.$$

Then let's consider this (for $i \neq j$)

$$a_i a_j|\psi\rangle = \psi_i\psi_j|\psi\rangle$$

But at the cost of a minus sign, we can also reverse the order of a_i and a_j before we let those act on the coherent state:

$$a_i a_j|\psi\rangle = -a_j a_i|\psi\rangle = -\psi_j\psi_i|\psi\rangle$$

Thus

$$\psi_i\psi_j = -\psi_j\psi_i$$

and at this point we could conclude that it is impossible to construct a coherent state for fermions, since ordinary numbers don't anticommute. But it turns out that there is a mathematical system of numbers, called the Grassmann numbers, that have exactly this property. We can use them to construct coherent states and out of that field integrals.

We introduce Grassmann variables by saying that first of all they anti-commute:

$$\psi_i\psi_j = -\psi_j\psi_i$$

This implies that the square of a Grassmann variable is 0:

$$\psi^2 = 0$$

Let's look at a function of a Grassmann number $f(\psi)$. We define this by inserting the ψ as the argument in the Taylor expansion of f. It turns out that such functions on Grassman variables have much less complexity than functions defined on ordinary numbers. Since the square of ψ is 0, we are left with only the constant and the first order term in ψ:

$$f(\psi) = f(0) + f'(0)\psi$$

Here $f(0)$ and $f'(0)$ are ordinary numbers and we will say that Grassmann variables commute with ordinary numbers.

We could also generalize this to functions of more variables. To define $f(\psi_1, \ldots, \psi_N)$, a multivariable function, one can expand f by the generalized Taylor expansion. Instead of giving the general formula (which we won't need) let us look at a particular case. Let's say we have a function of two variables $f(x, y)$ and we want the Grassmann version. Then we compute

$$f(\psi_1, \psi_2) = f(0,0) + \frac{\partial f}{\partial x}\bigg|_{x,y=0} \psi_1 + \frac{\partial f}{\partial y}\bigg|_{x,y=0} \psi_2 + \frac{\partial^2 f}{\partial x \partial y}\bigg|_{x,y=0} \psi_1\psi_2$$

All the other terms have higher powers of either ψ_1 or ψ_2 and therefore vanish.

Below we will need to define integrations over Grassmann variables. One of the properties that we have with ordinary integrals over the full domain to obey is this

$$\int dx \ f(x) = \int dx \ f(x + c)$$

(we use this with Gaussian integrals whenever we complete the square). We want the same to hold for Grassmann variables. In fact we can take that as the definition of Grassmann integrals. We know what the most general function of one variable is, so we plug it in and see:

$$\int d\psi \ f(\psi) = \int d\psi \ f(\psi + \psi')$$

Where ψ' is an arbitrary Grassmann number. The left hand side is $f(0) + f'(0)\psi$, while the right hand side is $\int d\psi \ f(0) + f'(0)(\psi + \psi')$. Equating these, we obtain

$$\int d\psi \ f'(0)\psi' = 0$$

Since ψ' is arbitray we have the rule

$$\int d\psi \ 1 = 0.$$

The product of two Grassmann variables commutes with any other Grassmann variables, since there are two minus signs involved. Thus we understand

the product of two Grassmann numbers as an ordinary number. Then $\int d\psi \, \psi$ is an ordinary number, which we define to be 1, which is a bit like a normalization of Grassmann numbers:

$$\int d\psi \, \psi = 1$$

How do Grassmann numbers behave when multiplied by a fermion operator? Let's take as an example the coherent state we want $a_j a_i |\psi\rangle = \psi_j \psi_i |\psi\rangle$, so:

$$a_j a_i |\psi\rangle = a_j (\psi_i |\psi\rangle) = -(\psi_i a_j |\psi\rangle) = -(\psi_i \psi_j |\psi\rangle) = (\psi_j \psi_i |\psi\rangle)$$

In the second equality we had to make a anticommute with ψ, otherwise would have obtained the wrong sign. Thus fermion operators and Grassmanns anticommute.

In this way we have constructed a logically consistent mathematical system and we can use it to build up our fermion coherent states. We construct similar to before

$$|\psi\rangle = \exp(\sum_i \psi_i a_i^+)|0\rangle.$$

But for the ket we can't just take the hermitian conjugate, since we don't have the notion of complex conjugation for Grassmann variables. They don't have a real and imaginary part. Thus we do something else instead, we introduce a ket that is independent of the bra and contains a new set of Grassmann variables that have a bar on top, but without the meaning that it's complex conjugation:

$$\langle\psi| = \langle 0| \exp(-\sum_i a_i \bar{\psi}_i) = \langle 0| \exp(\sum_i \bar{\psi}_i a_i)$$

With this we can state the completeness relation

$$\int d(\bar{\psi}, \psi) \, \exp(-\sum_i \bar{\psi}_i \psi_i)|\psi\rangle\langle\psi| = \mathbb{1},$$

where $\int d(\bar{\psi}, \psi) = \int \prod_i d\bar{\psi}_i d\psi_i$. Thus the only formal change here is the absence of the factor π in the measure. Now one can go through the whole steps similar to the ones we took for the bosonic states to prove the other useful facts about coherent states. These relations are unchanged.

Thus we have enough information now to construct the field integral for the partition function of fermions. Instead of repeating the steps, let us rather look at where the crucial differences are. The first step in our derivation was to insert a resolution of identity into

$$Z = \mathrm{Tr} e^{-\beta(H-\mu N)} = \sum_n \langle n|e^{-\beta(H-\mu N)}|n\rangle,$$

in order to get rid of the states $|n\rangle$. Let's do this:

$$Z = \sum_n \langle n|e^{-\beta(H-\mu N)}|n\rangle = \int d(\bar{\psi}, \psi) \, \exp(-\sum_i \bar{\psi}_i \psi_i) \sum_n \langle n|\psi\rangle\langle\psi|e^{-\beta(H-\mu N)}|n\rangle$$

One can prove that moving $\langle n|\psi\rangle$ to the right changes the sign of the Grassmann variables in one of the coherent states. Thus:

$$\langle n|\psi\rangle\langle\psi|m\rangle = \langle -\psi|m\rangle\langle n|\psi\rangle$$

This leads to

$$Z = \int d(\bar{\psi},\psi)\ \exp(-\sum_i \bar{\psi}_i\psi_i)\langle -\psi|e^{-\beta(H-\mu N)}|\psi\rangle$$

Now we can go through the same steps as before to derive the field integral for fermions. We obtain the same result with one very important difference: because we start with $\langle -\psi|e^{-\beta(H-\mu N)}|\psi\rangle$, ψ has to come back to $-\psi$ after at time $\hbar\beta$, i.e. the boundary condition on the field integral has changed:

$$Z = \int_{\psi(0)=-\psi(\beta\hbar)} D(\bar{\psi},\psi)e^{-\frac{1}{\hbar}S[\psi^*,\psi]} \tag{13}$$

with

$$S[\psi^*,\psi] = \int_0^{\beta\hbar} d\tau\,[\hbar\psi^*\partial_\tau\psi + H(\psi^*,\psi) - \mu N(\psi^*,\psi)]$$

Thus in this field integral approach to physics the only difference between bosons and fermions is a minus sign in the boundary conditions of the field integral and the use of complex vs. Graßmann variables. Bosons are periodic in imaginary time, while fermions are antiperiodic.