Quantum field theory in condensed matter

Martin Hohenadler
Institut für Theoretische Physik und Astrophysik
Universität Würzburg

Wintersemester 2015/16

1 Introduction

Want to describe condensed matter, which involves

- large numbers of particles ($\sim 10^{23}$ in solid state physics, $\sim 10^5$ in quantum simulators based on cold atomic gases)
- macroscopic quantum phenomena (coherence, Bose-Einstein condensate, superconductivity with a single wave function)
- often interested in cases with strong interactions between particles (Coulomb) that give rise to symmetry breaking (Mott insulator, magnetism). Not captured by perturbation theory.

Need methods to describe quantum mechanical many-particle systems.

Classical case:

- Few particles (classical mechanics): track $p_i(t)$, $q_i(t)$ of each particle via Newton's law, Hamiltonian or Lagrangian mechanics.
- Many particles (statistical mechanics): use macroscopic quantities like pressure, temperature, average energy instead. Microscopic details too complex, but also not crucial for comparison with experiment.

  temperature, pressure vary on much larger scales than distance between particles. Compare to electrodynamics, which is based on equations for electromagnetic fields.

Quantum case:

- Few particle (quantum mechanics): operators $\hat{p}_i(t)$, $\hat{q}_i(t)$, wave function, expectation values $\langle E \rangle$. Schrödinger equation.
- Many particles: complications

Theory of everything: (1D, single orbital in unit cell, spinless, clean)

$$
\begin{aligned}
H &= H_{\mathrm{e}} + H_{\mathrm{i}} + H_{\mathrm{ei}} \\
H_{\mathrm{e}} &= \sum_i \frac{p_i^2}{2m} + \sum_{i<j} V_{\mathrm{ee}}(r_i - r_j) \\
H_{\mathrm{i}} &= \sum_I \frac{P_I^2}{2M} + \sum_{I<J} V_{\mathrm{ii}}(R_I - R_J) \\
H_{\mathrm{ei}} &= \sum_{i,I} V_{\mathrm{ei}}(R_I - r_i)
\end{aligned}
$$

- Schrödinger equation typically cannot be solved exactly (numerics, variational ansatz, ...). Full knowledge typically not useful, because not accessible in experiment (compare to stat. mech.).
- particles cannot be distinguished (Heisenberg uncertainty relation implies that we cannot follow paths). Bose vs. Fermi statistics.
- Number of particles need not be conserved. $\Delta E \Delta t \geq \hbar/2$, and since energy can be converted to mass, we can have creation of particle-antiparticle pairs. Not captured by Schrödinger equation. Similarly, particles can be created/destroyed by interactions,

  $$H_I = \sum_{kq} V_q (a_q + a_{-q}^\dagger) c_{k+q}^\dagger c_k$$

  Similar: number of electrons may be constant, but number of fermions above/below Fermi level is not!

Here we will learn about methods from the realm of *Quantum Field Theory*, the most accurate and successful theory of physics. It was originally developed to combine electrodynamics (Maxwell's equations), quantum mechanics, and special relativity. *Quantum Electrodynamics*.

Key ideas and features:

- We know that electrons and photons can both behave like particles or waves. However, in classical physics, electrons are considered to be elementary, whereas light corresponds to wave excitations of the

electromagnetic field. To get a quantum theory, we have to resolve this difference.

Classical field theories resolve the problem of action at a distance (Newton) in terms of local fields $A(t, \vec{x})$ that mediate interactions.

From Quantum Mechanics, we know that we can get a quantum theory by replacing classical objects (position, momentum) by operators. Similarly, a quantum theory of light is based on quantizing the electromagnetic field.

Classical field: maps from spacetime to scalars, vectors, tensors
Quantum field: maps spacetime to scalar, vector, spinor operators.

In QFT, particles and waves correspond to excitations of quantum fields. For example, electron creation: $\psi^\dagger(\vec{x}, t)\,|0\rangle$. Because all electrons are excitations of the same field, they are identical!

In condensed matter physics, we use fields to describe low-energy excitations, which are potentially very different from electrons and ions. For example, 1D electrons can be described by field theory in terms of density waves using the method of bosonization.

- Interactions are described by scattering processes that involve particle creation and annihilation, as well as virtual (force) particles.
- Calculate scattering cross sections, amplitudes, correlation functions.
- Takes into account symmetries and symmetry breaking.

Here we mainly consider the path-integral formulation of QFT, based on integrating over paths/field configurations. Particularly powerful in the context of condensed matter physics, where many of the most interesting phenomena cannot be captured by perturbation theory (e.g., phase transitions, spontaneous symmetry breaking).

- Well-defined semi-classical limit, then take into account fluctuations.
- Fundamentally relativistic, in contrast to canonical quantization (see `https://en.wikipedia.org/wiki/Path_integral_formulation`).
- Allows to derive low-energy theories.

- Basis for stochastic numerical methods (Monte Carlo) because operators are replaced by numbers.

1.1 Hamilton's principle of least action

Whereas standard quantum mechanics is based on the Hamiltonian, QFT makes use of the Lagrangian formulation. In particular, the path-integral is closely related to Hamilton's principle of least action, which we review here. For simplicity, we mostly consider one spatial dimension.

Solving the differential equation corresponding to Newton's law of motion,

$$F = m\ddot{x}$$

gives us the path $x(t)$ of a particle at every time between $t = 0$ and some $t = \tau$. However, in quantum mechanics, paths are blurred by the uncertainty principle. Therefore, methods that try to calculate $x(t)$ seem inefficient.

Instead, for quantum systems we typically have the following situation:

- measure location/observable of a particle at $t = 0$ and $t = \tau$,

but do not know/care about evolution in between. Similar, in a scattering experiment, we can calculate/measure the amplitude $\langle q_1 q_2 \,|\, p_1 p_2 \rangle$.

Alternative approach for classical systems (Lagrange, Hamilton):

- Energy $E = T + V$ is conserved along the path $x(t)$ ($E = \overline{E}$), but balance between T and V will in general vary.
- Average kinetic energy:

$$\overline{T} = \frac{1}{\tau} \int_0^\tau \tfrac{1}{2} m[\dot{x}(t)]^2 \mathrm{d}t$$

- Average potential energy:

$$\overline{V} = \frac{1}{\tau} \int_0^\tau V[x(t)] \mathrm{d}t$$

$\overline{T}$, $\overline{V}$ depend on the whole path $x(t)$: *functionals*.
How do they change if we change the path? Answer: functional derivative.

Regular derivative:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{\epsilon\to 0} \frac{f(x+\epsilon) - f(x)}{\epsilon}$$

In general, the functional derivative of F can be defined as

$$\int \frac{\delta F}{\delta f}(x)\phi(x)\mathrm{d}x = \lim_{\epsilon\to 0} \frac{F[f+\epsilon\phi] - F[f]}{\epsilon}$$

with a test function $\phi(x)$ (interpret as scalar product, cf. $\nabla F \cdot \vec{\phi}$.)

For our purposes, it is sufficient to define the functional derivative as

$$\frac{\delta F[f(x)]}{\delta f(x_0)} = \lim_{\epsilon\to 0} \frac{F[f(x) + \epsilon\delta(x-x_0)] - F[f(x)]}{\epsilon}$$

= change of number $F[f(x_0)]$ upon variation of $f(x)$ at $x = x_0$. This works if the integrand can be expanded in a series to a least $\mathcal{O}(\epsilon)$.

- If the functional is an integral over a function, and we only change the path at one point, we need a δ function for a nontrivial effect.
- The change of F will in general depend on $f(x)$, the reference point for the variation, and on the point x_0 where we make the change.

Example 1: consider the functional derivative of $I[f] = \int_{-1}^{1} f(x)\mathrm{d}x$.

$$\begin{aligned}
\frac{\delta I[f]}{\delta f(x_0)} &= \lim_{\epsilon\to 0} \frac{1}{\epsilon}\left[\int_{-1}^{1} [f(x) + \epsilon\delta(x-x_0)] - \int_{-1}^{1} f(x)\mathrm{d}x\right] \\
&= \int_{-1}^{1} \delta(x-x_0)\mathrm{d}x \\
&= \begin{cases} 1 & x_0 \in [-1,1] \\ 0 & \text{else} \end{cases}
\end{aligned}$$

Example 2: We consider $H[f] = \int_a^b g[f(x)]\mathrm{d}x$, where g is a function and $g' = \mathrm{d}g/\mathrm{d}f$; $f(x)$ may correspond to a path $x(t)$.

$$\begin{aligned}\frac{\delta H[f]}{\delta f(x_0)} &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left[\int_a^b g[f(x)+\epsilon\delta(x-x_0)]\mathrm{d}x - \int_a^b g[f(x)]\mathrm{d}x\right] \\ &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left[\int_a^b \left(g[f(x)]+\epsilon\delta(x-x_0)g'[f(x)]\right)\mathrm{d}x - \int_a^b g[f(x)]\mathrm{d}x\right] \\ &= \int_a^b \delta(x-x_0)g'[f(x)]\mathrm{d}x \\ &= g'[f(x_0)]\end{aligned}$$

Hence, we obtain for the functional derivative of $\overline{V}$:

$$\frac{\delta\overline{V}[x]}{\delta x(t)} = \frac{1}{\tau}V'[x(t)]$$

Example 3: consider a functional $J[f] = \int g(f')\mathrm{d}y$ with $f' = \mathrm{d}f/\mathrm{d}y$.

$$\frac{\delta J[f]}{\delta f(x)} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left[\int_a^b \mathrm{d}y g\left(\frac{\partial}{\partial y}[f(y)+\epsilon\delta(y-x)]\right) - \int_a^b \mathrm{d}y g\left(\frac{\partial f}{\partial y}\right)\right]$$

The integrand of the first term can be expanded as

$$g\left(\frac{\partial}{\partial y}[f+\epsilon\delta(y-x)]\right) = g\left(f'+\epsilon\delta'(y-x)\right) \approx g(f') + \epsilon\delta'(y-x)\frac{\mathrm{d}g(f')}{\mathrm{d}f'}$$

Next, we integrate by parts, and assume that $x \in (a,b)$ so that $\delta(y-x) = 0$ at the integration limits $y = a, b$.

$$\begin{aligned}\frac{\delta J[f]}{\delta f(x)} &= \int_a^b \mathrm{d}y\delta'(y-x)\frac{\mathrm{d}g(f')}{\mathrm{d}f'} = \left[\delta(y-x)\frac{\mathrm{d}g(f')}{\mathrm{d}f'}\right]_a^b - \int_a^b \mathrm{d}y\delta(y-x)\frac{\mathrm{d}}{\mathrm{d}y}\frac{\mathrm{d}g(f')}{\mathrm{d}f'} \\ &= -\frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}g(f')}{\mathrm{d}f'}\end{aligned}$$

Applied to the average kinetic energy, we obtain

$$\frac{\delta\overline{T}[x]}{\delta x(t)} = -\frac{1}{\tau}m\ddot{x}$$

Since the force F in Newton's Law is simply $-V' = -\mathrm{d}V/\mathrm{d}x$ (more generally, $\vec{F} = -\nabla V$), the differential equation

$$F = \underbrace{-V'(x)}_{-\tau\frac{\delta\overline{V}}{\delta x}} = \underbrace{m\ddot{x}}_{-\tau\frac{\delta\overline{T}}{\delta x}}$$

which is equivalent to the condition

$$\frac{\delta\overline{V}[x]}{\delta x(t)} = \frac{\delta\overline{T}[x]}{\delta x(t)}\,.$$

Hence, if we deviate from $x(t)$, the average kinetic and potential energy change by equal amounts, and

$$\frac{\delta}{\delta x(t)}(\overline{T}[x] - \overline{V}[x]) = 0$$

on the classical path $x(t)$. The difference between T and V is called the Lagrangian,

$$L = T - V$$

and its time integral is called the action:

$$S = \int_0^\tau L\mathrm{d}t$$

For the case considered here, we further have

$$S = \int_0^\tau (T - V)\mathrm{d}t = \tau(\overline{T}[x] - \overline{V}[x])$$

so that $\frac{\delta}{\delta x(t)}(\overline{T}[x] - \overline{V}[x]) = 0$ is equivalent to

$$\frac{\delta S}{\delta x(t)} = 0$$

This equation is known as Hamilton's principle of least action, and states that the path taken by the particle is such that the action S is stationary.

From Hamilton's principle, we can derive the familiar Euler-Lagrange equation for the generalized coordinate x and its derivative $\dot{x}$ (velocity). Consider the change of S upon the variation $x \to x + \epsilon y$ (with $y = 0$ at $t = 0, \tau$):

$$\begin{aligned} S[x+\epsilon y] - S[x] &= \int \mathrm{d}t \left[L(x+\epsilon y, \dot{x}+\epsilon \dot{y}) - L(x,\dot{x}) \right] \\ &= \epsilon \int \mathrm{d}t \left[\frac{\partial L}{\partial x} y + \frac{\partial L}{\partial \dot{x}} \dot{y} \right] + \mathcal{O}(\epsilon^2) \\ &= \epsilon \int \mathrm{d}t \left[\frac{\partial L}{\partial x} y - \left(\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{x}} \right) y \right] + \left[\frac{\partial L}{\partial \dot{x}} y \right]_0^\tau + \mathcal{O}(\epsilon^2) \\ &= \epsilon \int \mathrm{d}t \left[\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{x}} \right] y + \mathcal{O}(\epsilon^2) \end{aligned}$$

Imposing $\epsilon^{-1}(S[x+\epsilon y] - S[x]) = 0$ for $\epsilon \to 0$ implies that

$$\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{x}} = 0 \tag{1}$$

Finally, it is common to define a Lagrangian density $\mathcal{L}$ via

$$L = \int \mathrm{d}x \mathcal{L}$$

in terms of which

$$S = \int \mathrm{d}t L = \int \mathrm{d}t \mathrm{d}x \mathcal{L}$$

To get used to the notation in the literature, let us now switch from paths $x(t)$ in one dimension to the case of configurations (paths) of a scalar field $\phi(x)$, where $x = (x^0, x^1, \ldots, x^m) = (t, \vec{x})$ is a point in m-dimensional spacetime. The action becomes

$$S = \int \mathrm{d}^m x \mathcal{L}(\phi, \partial_\mu \phi)$$

and the Euler-Lagrange equation takes the form

$$\frac{\delta S}{\delta \phi} = \frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \right) = 0 \tag{2}$$

Here, $\partial_\mu \phi = \partial \phi / \partial x^\mu = (\frac{\partial}{\partial t}, \nabla)\phi$.

In equation (1), the variation is with respect to the coordinate $x(t)$ itself. Here, the field ϕ depends on space and time, so we get time and space derivatives in the second term. An alternative way of writing equation (2) would be

$$\frac{\partial \mathcal{L}}{\partial \phi} - \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial(\partial\phi/\partial t)} - \sum_{k=1}^{m}\frac{\partial}{\partial x_k}\frac{\partial \mathcal{L}}{\partial(\partial\phi/\partial x_k)}$$

1.2 Harmonic oscillators

The problem of a quantum-mechanical harmonic oscillator and its generalizations provide a good starting point to understand several new concepts:

- Quantization of classical problems.
- Creation/annihilation operators, occupation number representation, Fourier transformation of operators.
- Collective degrees of freedom, continuum limit, fields.

1.2.1 Single oscillator

The Hamiltonian of the harmonic oscillator can be obtained by replacing the classical position and momentum variables with operators:

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega^2}{2}\hat{q}^2\,.$$

While this Hamiltonian is typically interpreted as describing a mass on a spring, it can also be seen as describing a special case of a particle with kinetic energy $p^2/2m$ moving in a potential $V(q) = \frac{1}{2}m\omega^2 q^2$. We have switched from the notation x for position to q in preparation for later.

The Schrödinger equation in real space takes the form ($\psi(q) = \langle q \,|\, \psi\rangle$)

$$\left[-\frac{1}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2}m\omega^2 q^2\right]\psi(q) = E\psi(q)$$

From QM, we know that a very efficient algebraic way of solving the problem is based on the introduction of operators

$$\begin{aligned} a &= \sqrt{\frac{m\omega}{2}}\left(\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p}\right) \\ a^\dagger &= \sqrt{\frac{m\omega}{2}}\left(\hat{q} - \frac{\mathrm{i}}{m\omega}\hat{p}\right) \end{aligned}$$

which is equivalent to

$$\begin{aligned} \hat{q} &= \sqrt{\frac{1}{2m\omega}}\left(a + a^\dagger\right) \\ \hat{p} &= -\mathrm{i}\sqrt{\frac{m\omega}{2}}\left(a - a^\dagger\right) \end{aligned}$$

Importantly, the new operators have the property

$$[a^\dagger, a^\dagger] = 0\,, \quad [a, a] = 0\,, \quad [a, a^\dagger] = 1\,,$$

and the Hamiltonian takes the form

$$\hat{H} = \omega\left(a^\dagger a + \tfrac{1}{2}\right)\,.$$

This form motivates to classify the eigenstates of the oscillator in terms of the number of excitation quanta of energy ω (phonons). If we denote a state with n excitations as $|n\rangle$, we can show that

$$a^\dagger a\,|n\rangle = \hat{n}\,|n\rangle = n\,|n\rangle\,.$$

The energy of such as state is $\omega(n + \frac{1}{2})$. The combination $a^\dagger a = \hat{n}$ is called the number operator.

Because

$$\begin{aligned} \hat{n}a^\dagger\,|n\rangle &= (n+1)a^\dagger\,|n\rangle \\ \hat{n}a\;\;|n\rangle &= (n-1)a\;\;|n\rangle \end{aligned}$$

the operators $a^\dagger$ and a are called creation and annihilation operators, respectively. In particular, we can create the eigenstate with n excitations and energy $\omega(n + \frac{1}{2})$ by applying the operator $a^\dagger$ to the ground state n times:

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

1.2.2 Independent oscillators

A formally trivial generalization of the harmonic oscillator paves the way to an efficient description of many-particle states. We consider a set of N independent oscillators (think of a one-dimensional crystal with lattice sites $i = 1, 2, \ldots, N$ where each site/unit cell has an internal lattice mode described by a harmonic oscillator):

$$\hat{H} = \sum_{k=1}^{N} \left(\frac{1}{2m} \hat{p}_j^2 + \frac{1}{2} m\omega^2 \hat{q}_j^2 \right) .$$

Because the oscillators are not coupled, we can solve them independently. In particular, we can write an eigenstate of the total system as a product state of the individual oscillators in the form

$$|n_1, n_2, n_3, \ldots, n_N\rangle = |n_1\rangle \otimes |n_2\rangle \otimes \cdots \otimes |n_N\rangle \ .$$

Let us define operators $a_k^\dagger$ and a_k that act only at the site of oscillator j:

$$a_j^\dagger \, |n_1, \ldots, n_j, \ldots, n_N\rangle \sim |n_1, n_2, \ldots, n_j + 1, \ldots, n_N\rangle$$
$$a_j \, |n_1, \ldots, n_j, \ldots, n_N\rangle \sim |n_1, n_2, \ldots, n_j - 1, \ldots, n_N\rangle$$

These operators have the property

$$[a_j^\dagger, a_k^\dagger] = 0 \, , \quad [a_j, a_k] = 0 \, , \quad [a_j, a_k^\dagger] = \delta_{jk}$$

and allow us to rewrite the Hamiltonian as

$$\hat{H} = \sum_j \omega \left(a_j^\dagger a_j + \tfrac{1}{2} \right)$$

(We could have allowed the potential to depend on j, so that $\omega \to \omega_j$.)

Finally, we can use the operators $a_j^\dagger$ and a_j to create (normalized!) *many-particle states* from the vacuum state $|0\rangle = |0, 0, \ldots, 0\rangle$ via

$$|\psi\rangle = |n_1, \ldots, n_j, \ldots, n_N\rangle = \frac{1}{\sqrt{n_1! n_2! \cdots n_N!}} (a_1^\dagger)^{n_1} (a_1^\dagger)^{n_2} \cdots (a_1^\dagger)^{n_N} \, |0\rangle \ .$$

The simple harmonic oscillator problem already reveals the possibility to describe a wave phenomenon (oscillations) in terms of abstract particles that are created with operators acting on a vacuum state $|0\rangle$.[1]

[1] The many-particle vacuum state is defined as the state that is destroyed by any annihilation operator, $a_k \, |0\rangle = 0$.

1.2.3 Coupled oscillators

So far, in the absence of any coupling between the different oscillators, the eigenstates of the system were simply product states of the individual oscillators. We now consider the case of coupled oscillators, described by

$$\hat{H} = \sum_j \left(\frac{\hat{p}_j^2}{2m} + \frac{K}{2}(\hat{q}_{j+1} - \hat{q}_j)^2 \right)$$

This looks more complicated than before because the oscillations of neighbouring oscillators are no longer independent!

To diagonalize the problem (obtain a form $\sum_k \omega_k a_k^\dagger a_k$), we first Fourier-transform to momentum space (the lattice constant is set to 1):[2]

$$\hat{q}_j = \frac{1}{\sqrt{N}} \sum_k \hat{q}_k \mathrm{e}^{\mathrm{i}kj} \qquad \hat{q}_k = \frac{1}{\sqrt{N}} \sum_j \hat{q}_j \mathrm{e}^{-\mathrm{i}kj}$$
$$\hat{p}_j = \frac{1}{\sqrt{N}} \sum_k \hat{p}_k \mathrm{e}^{\mathrm{i}kj} \qquad \hat{p}_k = \frac{1}{\sqrt{N}} \sum_j \hat{p}_j \mathrm{e}^{-\mathrm{i}kj}$$

On a periodic chain with N sites, the wave vector k can take on values $k = 2\pi n/N$, $n = 0, 1, \ldots, N-1$. We will also need the relation

$$\frac{1}{N} \sum_j \mathrm{e}^{\mathrm{i}j(k-p)} = \delta_{kp} \,.$$

Inserting the Fourier transform of $\hat{p}_j$ into the kinetic energy term, we have

$$\begin{aligned} \frac{1}{2m} \sum_j \hat{p}_j^2 &= \frac{1}{2m} \sum_j \left(\frac{1}{\sqrt{N}} \sum_k \hat{p}_k \mathrm{e}^{\mathrm{i}kj} \right) \left(\frac{1}{\sqrt{N}} \sum_{k'} \hat{p}_{k'} \mathrm{e}^{\mathrm{i}k'j} \right) \\ &= \frac{1}{2m} \sum_{k,k'} \hat{p}_k \hat{p}_{k'} \underbrace{\frac{1}{N} \sum_j \mathrm{e}^{\mathrm{i}j(k+k')}}_{\delta_{k,-k'}} = \frac{1}{2m} \sum_k \hat{p}_k \hat{p}_{-k} \end{aligned}$$

[2]Since we have a periodic (closed) chain, it is natural to assume the eigenmodes to be periodic in space. Periodic phenomena are best described by Fourier transformation.

For the potential energy term, we find

$$\begin{aligned}\frac{K}{2}\sum_j(\hat{q}_{j+1}-\hat{q}_j)^2 &= \frac{K}{2}\sum_j\left(\frac{1}{\sqrt{N}}\sum_k \hat{q}_k \mathrm{e}^{\mathrm{i}k(j+1)} - \frac{1}{\sqrt{N}}\sum_k \hat{q}_k \mathrm{e}^{\mathrm{i}kj}\right)^2 \\ &= \frac{K}{2}\frac{1}{N}\sum_j\left(\sum_k \hat{q}_k \mathrm{e}^{\mathrm{i}k(j+1)}\sum_{k'}\hat{q}_{k'}\mathrm{e}^{\mathrm{i}k'(j+1)} + \sum_k \hat{q}_k \mathrm{e}^{\mathrm{i}kj}\sum_{k'}\hat{q}_{k'}\mathrm{e}^{\mathrm{i}k'j}\right. \\ &\qquad \left. - \sum_k \hat{q}_k \mathrm{e}^{\mathrm{i}k(j+1)}\sum_{k'}\hat{q}_{k'}\mathrm{e}^{\mathrm{i}k'j} - \sum_{k'}\hat{q}_{k'}\mathrm{e}^{\mathrm{i}k'(j+1)}\sum_k \hat{q}_k \mathrm{e}^{\mathrm{i}kj}\right)\end{aligned}$$

which can be simplified to

$$\frac{K}{2}\sum_j(\hat{q}_{j+1}-\hat{q}_j)^2 = \frac{K}{2}\frac{1}{N}\sum_j\sum_{k,k'}\hat{q}_k\hat{q}_{k'}\left(\mathrm{e}^{\mathrm{i}j(k+k')}\mathrm{e}^{\mathrm{i}(k+k')} + \mathrm{e}^{\mathrm{i}j(k+k')} - \mathrm{e}^{\mathrm{i}j(k+k')}\mathrm{e}^{\mathrm{i}k} - \mathrm{e}^{\mathrm{i}j(k+k')}\mathrm{e}^{\mathrm{i}k'}\right)$$

and

$$\begin{aligned}\frac{K}{2}\sum_j(\hat{q}_{j+1}-\hat{q}_j)^2 &= \frac{K}{2}\frac{1}{N}\sum_j\sum_{k,k'}\hat{q}_k\hat{q}_{k'}\mathrm{e}^{\mathrm{i}j(k+k')}\left(\mathrm{e}^{\mathrm{i}(k+k')} + 1 - \mathrm{e}^{\mathrm{i}k} - \mathrm{e}^{\mathrm{i}k'}\right) \\ &= \frac{K}{2}\sum_{k,k'}\hat{q}_k\hat{q}_{k'}\underbrace{\frac{1}{N}\sum_j \mathrm{e}^{\mathrm{i}j(k+k')}}_{\delta_{k,-k'}}(\mathrm{e}^{\mathrm{i}k}-1)(\mathrm{e}^{\mathrm{i}k'}-1) \\ &= \frac{K}{2}\sum_k \hat{q}_k\hat{q}_{-k}(\mathrm{e}^{\mathrm{i}k}-1)(\mathrm{e}^{-\mathrm{i}k}-1)\end{aligned}$$

Using

$$(\mathrm{e}^{\mathrm{i}k}-1)(\mathrm{e}^{-\mathrm{i}k}-1) = 2-2\cos k = 2\cdot 2\sin^2(k/2) = 4\sin^2(k/2)$$

we can write

$$\frac{K}{2}\sum_j(\hat{q}_{j+1}-\hat{q}_j)^2 = \sum_k m\omega_k^2\,\hat{q}_k\hat{q}_{-k}$$

with the frequencies

$$\omega_k^2 = \frac{4K}{m}\sin^2(k/2)$$

Finally, we introduce creation and annihilation operators

$$a_k = \sqrt{\frac{m\omega_k}{2}} \left(\hat{q}_k + \frac{\mathrm{i}}{m\omega_k} \hat{p}_k \right)$$
$$a_k^\dagger = \sqrt{\frac{m\omega_k}{2}} \left(\hat{q}_{-k} - \frac{\mathrm{i}}{m\omega_k} \hat{p}_{-k} \right)$$

where we used $\hat{p}_k^\dagger = \hat{p}_{-k}$, $\hat{q}_k^\dagger = \hat{q}_{-k}$. In terms of these new operators, the Hamiltonian takes on the familiar diagonal form (exercise)

$$\hat{H} = \sum_k \omega_k \left(a_k^\dagger a_k + \tfrac{1}{2} \right) .$$

Even though we started with a set of coupled harmonic oscillators, we obtained a description in terms of independent particles that occupy energy levels k (corresponding to the wavevector). The particles describe collective excitations of the system and are called phonons. In the simple model we used, the phonons for different k are completely independent.

1.2.4 Continuum limit – field theory

Before moving on to second quantization, let us make first contact with field theory by considering the continuum limit of the coupled oscillator problem. The Hamiltonian was

$$\hat{H} = \sum_j \left(\frac{\hat{p}_j^2}{2m} + \frac{K}{2} (\hat{q}_{j+1} - \hat{q}_j)^2 \right) ,$$

where $\hat{p}_j$ and $\hat{q}_j$ are the momentum and displacement operators of an oscillator at lattice site j. We consider the classical case here, and return to the quantum problem later.

The motivation for a classical field theory is that the eigenmodes of the coupled oscillator problem are waves that involve all the lattice sites. In particular, because the energies scale as $\omega_k \sim |k|$ for small k, the low-energy excitations will have small k and hence long wavelengths. To describe such excitations, we usually do not have to worry about what happens on the scale of the lattice constant. Therefore, we can replace the vector of displacements

$\vec{\phi} = \{q_1(t), q_2(t), \ldots, q_N(t)\}$ by a continuous function $\phi(x,t)$.[3] Instead of field theory, one sometimes also speaks of a hydrodynamical approach.

The continuum limit works as follows:

- Consider a periodic chain of masses with lattice constant a and total length (=volume) $V = Na$. We want to take the limits $a \to 0$ and $N \to \infty$ (we add more and more masses, but reduce their distance) with $Na = V = \text{const}$.
- For the kinetic term, we write $p_i = m\partial_t q_i$, so that

  $$\frac{p_j^2}{2m} \mapsto \frac{1}{2} m \left(\frac{\partial q_j}{\partial t}\right)^2$$

  For $a \to 0$, we have ($a \sum_j \mapsto \int \mathrm{d}x$)

  $$a \sum_j \frac{1}{2} \frac{m}{a} \left(\frac{\partial q_j}{\partial t}\right)^2 \mapsto \int \mathrm{d}x \frac{1}{2} \rho \left(\frac{\partial \phi}{\partial t}\right)^2$$

  where $\rho = m/a$ is the mass density of the system (originally, we had a mass m per lattice constant a, and we want to keep that ratio fixed).
- For the potential term, we have ($\tau = Ka$ is the string tension)

  $$a \sum_j \frac{1}{2} Ka \left(\frac{q_{j+1} - q_j}{a}\right)^2 \mapsto \int \mathrm{d}x \frac{1}{2} \tau \left(\frac{\partial \phi}{\partial x}\right)^2$$

The continuum limit of the Hamiltonian is therefore given by

$$H = T + V = \int \mathrm{d}x \left[\frac{1}{2} \rho \left(\frac{\partial \phi}{\partial t}\right)^2 + \frac{1}{2} \tau \left(\frac{\partial \phi}{\partial x}\right)^2\right]$$

whereas the Lagrangian takes the form

$$L = T - V = \int \mathrm{d}x \left[\frac{1}{2} \rho \left(\frac{\partial \phi}{\partial t}\right)^2 - \frac{1}{2} \tau \left(\frac{\partial \phi}{\partial x}\right)^2\right] = \int \mathrm{d}x \mathcal{L}$$

[3] $\phi(x,t)$ is a classical scalar field, a mapping $(x,t) \to \phi(x,t) \in \mathbb{R}$. Generally, in field theory, the position x appears as a label rather than as a dynamic variable.

The Lagrangian gives us a description of our original problem of coupled oscillators in terms of the field ϕ, so we have our first field theory.

To solve the continuum theory, we can use Hamilton's principle, which is of course equivalent to the Euler-Lagrange equation. Imposing a stationary action, we find

$$\begin{aligned}
0 = \frac{\delta S}{\delta \phi} &= \frac{\partial \mathcal{L}}{\partial \phi} - \frac{\partial}{\partial x}\frac{\partial \mathcal{L}}{\partial(\partial\phi/\partial x)} - \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial(\partial\phi/\partial t)} \\
&= 0 - \frac{\partial}{\partial x}\frac{\partial}{\partial(\partial\phi/\partial x)}\left[-\frac{1}{2}\tau\left(\frac{\partial\phi}{\partial x}\right)^2\right] - \frac{\partial}{\partial t}\frac{\partial}{\partial(\partial\phi/\partial t)}\left[\frac{1}{2}\rho\left(\frac{\partial\phi}{\partial t}\right)^2\right] \\
&= \tau\frac{\partial}{\partial x}\left(\frac{\partial\phi}{\partial x}\right) - \rho\frac{\partial}{\partial t}\left(\frac{\partial\phi}{\partial t}\right) \\
&= \tau\frac{\partial^2\phi}{\partial x^2} - \rho\frac{\partial^2\phi}{\partial t^2}\,.
\end{aligned}$$

Hence, the Euler-Lagrange equation gives us the 1D wave equation

$$\frac{\partial^2\phi}{\partial t^2} = \underbrace{\frac{\tau}{\rho}}_{c^2}\frac{\partial^2\phi}{\partial x^2}$$

which we can solve to obtain the allowed eigenmodes and wavevectors. The general solution can be written as a superposition $\phi(x,t) = \sum_{k_n} a_{k_n} \mathrm{e}^{-\mathrm{i}(\omega t - k_n x)}$.

We have hence solved a classical many-body problem (as compared to typical classical mechanics problems) using Hamilton's least action principle in terms of the collective modes rather than the underlying lattice problem. A similar approach can be used for other problems, both classical and quantum.

2 Lagrangians and canonical quantization

2.1 Examples of scalar field theories

The above example has shown how we can start from a microscopic description/model, and derive a field theory for the low-energy physics. This approach to many-body problems is very useful. Since classical Lagrangians often serve as the starting point for the description of quantum mechanical systems, let us consider some important examples.

2.1.1 Massless scalar field

$$\mathcal{L} = \frac{1}{2}\partial^\mu\phi\partial_\mu\phi = \frac{1}{2}(\partial_\mu\phi)^2 = \frac{1}{2}(\partial_0\phi)^2 - \frac{1}{2}\nabla\phi\cdot\nabla\phi$$

For the Euler-Lagrange equations, we need the derivatives

$$\frac{\partial\mathcal{L}}{\partial\phi} = 0\,, \quad \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)} = \partial^\mu\phi$$

and the d'Alembertian operator[4]

$$\partial^2 = \partial^\mu\partial_\mu = \partial_\mu\partial^\mu = \frac{\partial^2}{\partial t^2} - \nabla^2 = \frac{\partial^2}{\partial t^2} - \Delta = \Box$$

and find the equation of motion for the field

$$\partial_\mu\partial^\mu\phi = \frac{\partial^2\phi}{\partial t^2} - \Delta\phi = 0$$

which is just the 3D analogue of the wave equation with $c = 1$. The solutions have a wavevector dependent energy $\omega = E_{|\vec{p}|} = c|\vec{p}|$. A dispersion relation with $E_0 = 0$ (corresponding to a vanishing minimal energy) is referred to as gapless or massless.

[4]We have $\partial_\mu = (\partial_0, \nabla)$ and $\partial^\mu = (\partial_0, -\nabla)$.

2.1.2 Massive scalar field

To obtain a massive spectrum, we can add a mass term (a potential energy for the field). From the Lagrangian

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)^2 - \frac{1}{2}m^2\phi^2$$

and

$$\frac{\partial \mathcal{L}}{\partial \phi} = -m^2\phi\,, \quad \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} = \partial^\mu \phi$$

we obtain the Klein-Gordon equation

$$(\partial_\mu \partial^\mu + m^2)\phi = 0$$

which describes free relativistic particles (plane waves) with energy $E_{\vec{p}} = \vec{p}^2 + m^2$. The Klein-Gordon equation is also the relativistic generalization of the Schrödinger equation for free spinless particles.

2.1.3 Adding an external source

The simplest way to add interactions is to consider an external source $J(x)$ that creates a disturbance/excitation of the field at point x. The corresponding Lagrangian takes the form

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)^2 - \frac{1}{2}m^2\phi^2 + J(x)\phi(x)$$

and the equation of motion becomes

$$(\partial_\mu \partial^\mu + m^2)\phi(x) = J(x)\,.$$

2.1.4 Adding interactions: ϕ^4 theory

Finally, let us write down a simple yet nontrivial interacting theory,

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)^2 - \frac{1}{2}m^2\phi^2 - \frac{1}{4!}\lambda\phi^4$$

which cannot be solved exactly, and describes for example the physics of the Ising model (a lattice model of spins with values $s_i = \pm 1$, in 1D we have $H = J\sum_i s_{i+1}s_i + h\sum_i s_i$) close to the magnetic transition. The parameter λ is the interaction strength.

To see how such a Lagrangian can describe symmetry breaking, we generalize it to

$$\mathcal{L} = \frac{1}{2}(\partial_\mu\phi)^2 - \frac{1}{2}\alpha\phi^2 - \frac{1}{4}\lambda\phi^4 = \frac{1}{2}(\partial_\mu\phi)^2 - U(\phi)$$

with the potential $U(\phi)$. Here, α is a temperature dependent parameter, and $\lambda > 0$. We consider $\alpha \sim T - T_c$ so that we have a sign change at a critical temperature T_c. For $T > T_c$, the potential $U(\phi)$ has a single minimum at $\phi = 0$. However, for $T < T_c$, the potential has a maximum at $\phi = 0$ and minima at $\phi_0 = \pm\sqrt{-\alpha/\lambda}$. At low temperatures, the field will therefore have a nonzero vacuum expectation value $\langle 0|\,\phi\,|0\rangle = \phi_0$. The Lagrangian is still symmetric under the discrete transformation $\phi \to -\phi$, but the ground state will break this symmetry spontaneously by selecting one of the two minima. The use of an effective Lagrangian to model physical phenomena is known under the name Landau-Ginzburg theory, where the free energy is expanded in powers of the order parameter. The fact that microscopically different phenomena (magnetism, superconductivity) can be described by the same Lagrangian is called universality, and lies at the heart of statistical physics. Crucially, the behaviour of the system close to a second-order phase transition depends only on the dimension and the symmetry of the order parameter/field. For example, the order parameter in the ordered phase behaves as $\langle\phi\rangle \sim (-\tau)^\beta$ with $\tau = (T - T_c)/T_c$, where β is one of the critical exponents ($\beta = 1/2$ for a mean-field-like transition).

2.1.5 Complex scalar field theory

So far, we have only considered real scalar fields. The type of field depends on the physics we want to describe. A real scalar field is sufficient to describe for example lattice displacements. On the other hand, the momentum eigenstates of the Klein-Gordon equation are in general complex (plane waves). Another example of a complex field is the order parameter of a superconductor. The Lagrangian of a complex scalar field theory with interactions is

given by

$$\mathcal{L} = \partial^\mu \psi^\dagger \partial_\mu \psi - m^2 \psi^\dagger \psi - \lambda (\psi^\dagger \psi)^2$$

The complex field is equivalent to two coupled scalar fields

$$\psi^\dagger = \frac{1}{\sqrt{2}}(\phi_1 + \mathrm{i}\phi_2)\,, \quad \psi \ = \frac{1}{\sqrt{2}}(\phi_1 - \mathrm{i}\phi_2)\,.$$

The real and imaginary part of ψ are independent degrees of freedom.

2.2 Canonical quantization

While we will mostly focus on the path-integral formalism in this course, it is important to mention the process of canonical quantization. Starting from a classical Lagrangian density $\mathcal{L}$ for a real scalar field canonical quantization proceeds as follows toward a quantum field theory:

1. Obtain the momentum density defined as $\Pi^0(x) = \partial\mathcal{L}/\partial(\partial_0\phi)$, and the Hamiltonian density via Legendre transformation: $\mathcal{H} = \Pi^0 \partial_0 \phi - \mathcal{L}$.

2. Quantize the fields by imposing equal-time commutation relations

   $$[\hat{\phi}(x), \hat{\Pi}^0(y)] = \mathrm{i}\delta^{(3)}(\vec{x} - \vec{y})$$

   The fields are the counterparts of position and momentum in quantum mechanics, where $[\hat{x}, \hat{p}] = \mathrm{i}\hbar$.[5] We want a local theory where the measurement of a field at x is independent of a measurement at $y \neq x$.

3. Express the quantum fields in terms of creation/annihilation operators $a_{\vec{p}}, a^\dagger_{\vec{p}}$, then express the Hamiltonian in terms of $a_{\vec{p}}, a^\dagger_{\vec{p}}$.

2.2.1 Coupled oscillators

In fact, we have already carried out many of these steps (but in different order) for the coupled oscillator problem. The Lagrangian of our problem

[5] In classical mechanics, the canonical momentum is $p_i = \partial L/\partial \dot{q}_i$. The field-theory analogue is $\pi(x) = \partial\mathcal{L}/\partial\dot{\phi}$. A four-vector suitable for 3+1 dimensions is $\Pi_\mu(x) = \partial\mathcal{L}/\partial(\partial_\mu\phi)$.

ended up to be (step 0, write down Lagrangian)

$$\mathcal{L} = \tfrac{1}{2}\rho \left(\frac{\partial\phi}{\partial t}\right)^2 - \tfrac{1}{2}\tau \left(\frac{\partial\phi}{\partial x}\right)^2 .$$

If we set $\tau = \mu = 1$ ($c = 1$), we can write $\mathcal{L}$ in the Lorentz-invariant form

$$\mathcal{L} = \tfrac{1}{2}(\partial_\mu\phi)^2$$

which is identical to the free scalar bosonic field theory above. $\mathcal{L}$ is related to the Hamiltonian (we work in the continuum limit)

$$H = \tfrac{1}{2}\int \mathrm{d}x \left([\partial_0\phi]^2 + [\partial_x\phi]^2\right) .$$

The canonical momentum field is given by $\Pi_\mu(x,t) = \partial_\mu\phi(x,t)$. Hence, the first term in H is related to Π_0. Step 2 consists of promoting the classical fields ϕ and Π to operators by imposing $[\hat{\phi}(x), \hat{\Pi}^0(y)] = \mathrm{i}\delta^{(3)}(\vec{x} - \vec{y})$. Finally, we have to express the field operators in terms of creation/annihilation operators. For the coupled oscillator problem, we had

$$\hat{q}_k = \sqrt{\frac{1}{2m\omega_k}} \left(a_k + a_{-k}^\dagger\right)$$

or in real space (we want a quantum field $\hat{\phi}(x,t)$)

$$\hat{q}_j = \frac{1}{\sqrt{N}} \sum_k \hat{q}_k \mathrm{e}^{\mathrm{i}kj} = \sum_k \frac{1}{\sqrt{2m\omega_k N}} \left(a_k \mathrm{e}^{\mathrm{i}kj} + a_k^\dagger \mathrm{e}^{-\mathrm{i}kj}\right)$$

and including time dependence

$$\hat{q}_j(t) = \mathrm{e}^{\mathrm{i}\hat{H}t} \hat{q}_j \mathrm{e}^{-\mathrm{i}\hat{H}t} = \sum_k \frac{1}{\sqrt{2m\omega_k N}} \left(a_k \mathrm{e}^{-\mathrm{i}(E_k t - kj)} + a_k^\dagger \mathrm{e}^{\mathrm{i}(E_k t - kj)}\right) .$$

In the continuum limit, we replace $\hat{q}_j(t)$ with a field $\phi(x,t)$ and ω_k by a general dispersion E_k to get

$$\hat{\phi}(x,t) \sim \int \mathrm{d}k \frac{1}{\sqrt{E_k}} \left(a_k \mathrm{e}^{-\mathrm{i}(E_k t - kj)} + a_k^\dagger \mathrm{e}^{\mathrm{i}(E_k t - kj)}\right)$$

The canonical momentum is given by

$$\hat{\Pi}_0 = \partial_0\hat{\phi}(x,t) \sim \int \mathrm{d}k \frac{1}{\sqrt{E_k}} (-\mathrm{i}E_k) \left(a_k \mathrm{e}^{-\mathrm{i}(E_k t - kj)} + a_k^\dagger \mathrm{e}^{\mathrm{i}(E_k t - kj)}\right)$$

and the Hamiltonian becomes

$$\hat{H} = \int \mathrm{d}k E_k \left(a_k^\dagger a_k + \tfrac{1}{2}\right)$$

2.2.2 Complex scalar field theory

We consider the complex field theory (step 0; x is the four vector)

$$\mathcal{L} = \partial^\mu \psi^\dagger(x) \partial_\mu \psi(x) - m^2 \psi^\dagger(x) \psi(x) \,.$$

For each component $\sigma = \psi^\dagger, \psi$ we determine the corresponding momentum:[6]

$$\Pi^0_\psi \;= \frac{\partial \mathcal{L}}{\partial(\partial_0 \psi)} = \partial^0 \psi^\dagger = \partial_0 \psi^\dagger \,, \quad \Pi^0_{\psi^\dagger} = \frac{\partial \mathcal{L}}{\partial(\partial_0 \psi^\dagger)} = \partial^0 \psi \;= \partial_0 \psi$$

The Hamiltonian density follows from the Legendre transformation

$$\begin{aligned}
\mathcal{H} &= \sum_\sigma \Pi^0_\sigma \partial_0 \sigma - \mathcal{L} \\
&= \partial_0 \psi^\dagger \partial_0 \psi \;+ \partial_0 \psi \;\partial_0 \psi^\dagger - (\partial_0 \psi^\dagger \partial_0 \psi - \nabla \psi^\dagger \cdot \nabla \psi \;- m^2 \psi^\dagger \psi) \\
&= \partial_0 \psi^\dagger \partial_0 \psi \;+ \nabla \psi^\dagger \cdot \nabla \psi \;+ m^2 \psi^\dagger \psi
\end{aligned}$$

Step 3 consists of making the classical fields into quantum fields by imposing commutation relations between the fields and the momenta,

$$\left[\hat{\psi}(\mathbf{x}, t), \hat{\Pi}^0_\psi \;(\mathbf{y}, t)\right] = \left[\hat{\psi}^\dagger(\mathbf{x}, t), \hat{\Pi}^0_{\psi^\dagger}(\mathbf{y}, t)\right] = \mathrm{i}\delta^{(3)}(\mathbf{x} - \mathbf{y})$$

and expanding the field operators in terms of creation and annihilation operators. Because the complex field has two degrees of freedom, we need two sets of operators $a^\dagger, a$ and $b^\dagger, b$ instead of just one:[7]

$$\begin{aligned}
\hat{\psi}(x) &= \int \frac{\mathrm{d}^3 p}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_\mathbf{p}}} \left(a_\mathbf{p} \, \mathrm{e}^{-\mathrm{i}p\cdot x} + b^\dagger_\mathbf{p} \, \mathrm{e}^{\mathrm{i}p\cdot x}\right) \\
\hat{\psi}^\dagger(x) &= \int \frac{\mathrm{d}^3 p}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_\mathbf{p}}} \left(a^\dagger_\mathbf{p} \, \mathrm{e}^{\mathrm{i}p\cdot x} + b_\mathbf{p} \, \mathrm{e}^{-\mathrm{i}p\cdot x}\right)
\end{aligned}$$

Here, $E_\mathbf{p} = +\sqrt{\mathbf{p}^2 + m^2}$ is the free-particle dispersion, and we have the nonzero commutation relations

$$[a_\mathbf{p}, a^\dagger_\mathbf{q}] = [b_\mathbf{p}, b^\dagger_\mathbf{q}] = \delta^{(3)}(\mathbf{p} - \mathbf{q})$$

[6] Remember that for the time component $\partial_0 = \partial^0$ since in the metric tensor $g_{00} = 1$.

[7] The prefactor $(2\,E_\mathbf{p})^{-1/2}$ follows from the requirement of Lorentz invariance.

The physical interpretation here is that $a^\dagger, a$ describe particles, and $b^\dagger, b$ antiparticles. Finally, we insert the expansion into $\hat{\mathcal{H}}$ to obtain after simplification and normal-ordering

$$\mathrm{N}[\hat{H}] = \int \mathrm{d}^3 p \, E_{\mathbf{p}} \left(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + b^\dagger_{\mathbf{p}} b_{\mathbf{p}} \right)$$

2.2.3 Comments on canonical quantization

- The form of the mode expansion of the field in terms of creation and annihilation operators depends on the field theory (scalar vs. vector, real vs. complex, ...).
- In general, we first end up with a Hamiltonian that contains terms $a^\dagger a + a a^\dagger = 2a^\dagger a + \delta(0)$. To avoid an infinite energy, we can impose normal ordering, with all creation operator left of all annihilation operators.
- The choice of Lagrangian is usually dictated by the problem at hand, and by the symmetries of the field that determine which types of terms can be present in $\mathcal{L}$. For example, Lorentz invariance implies no derivatives of higher order than first. Quite often, we know that we want to describe a certain phenomenon (e.g., spontaneous symmetry breaking in a magnet), and can write down a classical Lagrangian that captures the corresponding physics.
- Of course, for problems that are not quadratic (i.e., harmonic oscillators), the resulting field theory has not been solved at this point. Quantum effects enter here via the commutation relations between fields.
- In condensed matter physics, we quite often start with a Hamiltonian that models a certain material (or important aspects of it), and then derive a field theory description via the path integral.

2.3 Non-relativistic regime – condensed matter

Starting from the complex field theory, we can take the non-relativistic limit usually encountered in condensed matter physics. To this end, we notice that the energy of slow particles takes the form $E = mc^2 + \epsilon$ with ϵ small. Remember that in quantum mechanics, the time dependence of eigenstates follows from the Schrödinger equation $\mathrm{i}\hbar\partial_t\psi = E\psi$, which can be integrated to get $\psi(t) = \psi(0)\mathrm{e}^{-\mathrm{i}Et}$. If E is dominated by the rest mass, the fast oscillations will mask any interesting dynamics on longer time scales. To factor out the uninteresting dynamics related to the rest mass, let us transform the field according to (we set $\hbar$ and c equal to 1 again, and add a useful prefactor)

$$\psi \mapsto \frac{1}{\sqrt{2m}}\mathrm{e}^{-\mathrm{i}mt}\psi\,.$$

Inserting the transformed field into $\mathcal{L}$ we obtain

$$\begin{aligned}\mathcal{L} &= (\partial_0\psi^\dagger)(\partial_0\psi) - \nabla\psi^\dagger\cdot\nabla\psi - m^2\psi^\dagger\psi - \lambda(\psi^\dagger\psi)^2 \\ &= \frac{1}{2m}\left\{\left[(\partial_0 + \mathrm{i}m)\psi^\dagger\right]\left[(\partial_0 - \mathrm{i}m)\psi\right] - \nabla\psi^\dagger\cdot\nabla\psi - m^2\psi^\dagger\psi - \frac{\lambda}{2m}(\psi^\dagger\psi)^2\right\}\,.\end{aligned}$$

Let us consider only the first and the third term, which can be written as

$$\partial_0\psi^\dagger\partial_0\psi + \mathrm{i}m[\psi^\dagger\partial_0\psi + (\partial_0\psi^\dagger)\psi] + m^2\psi^\dagger\psi - m^2\psi^\dagger\psi$$

The last two terms cancel. The first term is a factor m smaller than the second, and can hence be neglected. Finally, we can integrate by parts[8] to show that $(\partial_0\psi^\dagger)\psi = -\psi^\dagger\partial_0\psi$. Therefore, we have in total

$$\mathcal{L} = \mathrm{i}\psi^\dagger\partial_0\psi - \frac{1}{2m}\nabla\psi^\dagger\cdot\nabla\psi - \frac{g}{2}(\psi^\dagger\psi)^2$$

with $g = \lambda/2m^2$. Clearly, if our system is not relativistic, the Lagrangian looks much less symmetric.

While in high-energy physics the density of particles is typically zero, condensed matter systems have a finite density of electrons, bosons, etc., corresponding to a nonzero value of $\psi^\dagger\psi$ in the ground state. We can take this fact into account by adding an average density

$$\mathcal{L} = \mathrm{i}\psi^\dagger\partial_0\psi - \frac{1}{2m}\nabla\psi^\dagger\cdot\nabla\psi - \frac{g}{2}(\psi^\dagger\psi - \overline{\rho})^2\,.$$

[8] Remember that ultimately we are interested in an action $S = \int \mathrm{d}x\mathrm{d}t\mathcal{L}$.

Both the relativistic and the non-relativistic complex scalar theories are invariant under the continuous $U(1)$ symmetry transformation

$$\psi \mapsto \psi \mathrm{e}^{\mathrm{i}\alpha}\,, \quad \psi^\dagger \mapsto \psi^\dagger \mathrm{e}^{-\mathrm{i}\alpha}\,.$$

It is instructive to rewrite the field in the form

$$\psi = \sqrt{\rho(x)}\,\mathrm{e}^{\mathrm{i}\theta(x)}\,,$$

so that the symmetry becomes a symmetry under $\theta \mapsto \theta + \alpha$. We can express $\mathcal{L}$ in terms of the new variables ρ and θ:

$$\begin{aligned}
\mathcal{L} &= \mathrm{i}\sqrt{\rho(x)}\mathrm{e}^{-\mathrm{i}\theta(x)}\partial_0\sqrt{\rho(x)}\mathrm{e}^{\mathrm{i}\theta(x)} - \frac{1}{2m}\nabla\sqrt{\rho(x)}\mathrm{e}^{-\mathrm{i}\theta(x)}\cdot\nabla\sqrt{\rho(x)}\mathrm{e}^{\mathrm{i}\theta(x)} - \frac{g}{2}\rho^2 \\
&= \mathrm{i}\sqrt{\rho(x)}\mathrm{e}^{-\mathrm{i}\theta(x)}\left[\frac{1}{2\sqrt{\rho}}(\partial_0\rho)\mathrm{e}^{\mathrm{i}\theta} + \mathrm{i}\sqrt{\rho}\mathrm{e}^{\mathrm{i}\theta}\partial_0\theta\right] - \frac{g}{2}\rho^2 \\
&\quad - \frac{1}{2m}\left[\mathrm{e}^{-\mathrm{i}\theta}\frac{1}{2\sqrt{\rho}}\nabla\rho + \sqrt{\rho}(-\mathrm{i}\nabla\theta)\mathrm{e}^{-\mathrm{i}\theta}\right]\cdot\left[\mathrm{e}^{\mathrm{i}\theta}\frac{1}{2\sqrt{\rho}}\nabla\rho + \sqrt{\rho}(\mathrm{i}\nabla\theta)\mathrm{e}^{\mathrm{i}\theta}\right] \\
&= \tfrac{1}{2}\mathrm{i}\partial_0\rho - \rho\partial_0\theta - \frac{1}{2m}\left[\frac{1}{4\rho}(\nabla\rho)^2 + \rho(\nabla\theta)^2\right] - \frac{g}{2}\rho^2
\end{aligned}$$

The canonical momenta are given by

$$\begin{aligned}
\Pi^0_\rho(x) &= \frac{\partial\mathcal{L}}{\partial(\partial_0\rho)} = \frac{\mathrm{i}}{2} \\
\Pi^0_\theta(x) &= \frac{\partial\mathcal{L}}{\partial(\partial_0\theta)} = -\rho
\end{aligned}$$

Quantizing the field θ and its conjugate momentum in the form

$$[\hat{\theta}(x), \hat{\Pi^0_\theta}(y)] = [\hat{\theta}(x), -\hat{\rho}(x)] = [\hat{\rho}(x), \hat{\theta}(x)] = \mathrm{i}\delta^{(3)}(\vec{x} - \vec{y})$$

and integrating over space, we find the number-phase uncertainty relation

$$[\hat{N}, \hat{\theta}] = \mathrm{i}$$

which reveals that phase and particle number are conjugate variables. For example, if a superconductor has a well-defined phase of the order parameter, the uncertainty in the particle number is large, and vice versa.

According to Noether's Theorem, the invariance of $\mathcal{L}$ under the continuous symmetry transformation $\theta \mapsto \theta + \delta\alpha$, that is $\delta\mathcal{L} = 0$, implies that if the fields fulfil the Euler-Lagrange equations (so that the action is stationary) the Noether current

$$J^\mu_{\mathrm{N}} = -\Pi^\mu_\theta = (J^0_{\mathrm{N}}, \vec{J}_{\mathrm{N}}) = \left(\rho, \frac{\rho}{m}\nabla\theta\right)$$

is locally conserved

$$\partial_\mu J^\mu_{\mathrm{N}} = 0\,,$$

which is equivalent to the continuity equation

$$\partial_t J^0_{\mathrm{N}} + \nabla \cdot \vec{J}_{\mathrm{N}} = \partial_t \rho + \nabla \cdot \vec{J}_{\mathrm{N}} = 0$$

Therefore, the Noether charge

$$Q_{\mathrm{N}} = \int \mathrm{d}^3x J^0_{\mathrm{N}} = \int \mathrm{d}^3x \rho = N$$

is conserved since

$$\frac{\mathrm{d}Q_{\mathrm{N}}}{\mathrm{d}t} = \int \mathrm{d}^3x \partial_0 J^0_{\mathrm{N}} = -\int \mathrm{d}^3x \nabla \cdot \vec{J}_{\mathrm{N}} = -\int \mathrm{d}\vec{S} \cdot \vec{J}_{\mathrm{N}} = 0\,,$$

where the last step follows if we assume that the current density vanishes on the surface S of integration.

3 Feynman's path integral

3.1 Simple derivation

A central concept of quantum mechanics as compared to classical mechanics is the probabilistic interpretation. Classically, the system is in a state uniquely determined by $q(t)$, $p(t)$ at each time t, and the value of an observable $A(q,p)$ (a function of q, p) is simply $A(q(t),p(t))$. In quantum mechanics, the state of the system is described by a state vector $|\psi\rangle$. Observables correspond to Hermitian operators with real eigenvalues a_m and eigenstates $|\phi_m\rangle$, and may be expressed in terms of the operators $\hat{q}$, $\hat{p}$. A measurement of $\hat{A}$ will give one of the eigenvalues of $\hat{A}$. The probability to obtain the eigenvalue a_m is given by $|\langle m \,|\, \psi\rangle|^2$, where $\langle m \,|\, \psi\rangle$ is known as the probability amplitude. If we consider the position operator $\hat{Q}$, $\langle q \,|\, \psi\rangle$ is the wave function $\psi(q)$.

For example in a scattering experiment (particle physics, but also photoemission) we may consider the amplitude

$$\langle q_b, t_b \,|\, q_a, t_a\rangle$$

for a particle to start at position q_a at time t_a, and end up at position q_b at a later time t_b, which is usually called the propagator. Clearly, the value $\langle q_b, t_b \,|\, q_a, t_a\rangle$ depends on the path taken between q_a and q_b. Classically, we know that the path will be determined by the Euler-Lagrange equation, the solution of which minimizes the action

$$S = \int_{t_a}^{t_b} \mathrm{d}t L\,.$$

Feynman discovered that quantum mechanically, a particle moving between q_a and q_b will take every possible path, and that each path is associated with a phase factor $\mathrm{e}^{\mathrm{i}S/\hbar}$ where S is the classical action. The first part can in fact be easily understood from double-slit experiments. If we have two slits A_1 and A_2 in a single screen A, the amplitude for a particle to start at q_a and be found at q_b on the detector is $G(q_b,q_a) = G(q_b,A_1)G(A_1,q_a) + G(q_b,A_2)G(A_2,q_a)$. If we add more slits, we end up with $G(q_b,q_a) = \sum_i G(q_b,A_i)G(A_i,q_a)$. Let us now add a second screen B between A and the detector. Clearly, $G(q_b,q_a) = \sum_i \sum_j G(q_b,B_j)G(B_j,A_i)G(A_i,q_a)$. Finally, if we add more and

more screens, we find (we will become more precise in a minute)

$$G(q_b, q_a) \sim \sum_{\text{slits}} \prod_{\text{screens}} G(q_{n+1}, q_n)\,.$$

Because an infinite number of screens with an infinite number of slits is identical to no screens at all, the amplitude $G(q_b, q_a)$ should be the sum over all possible paths that the particle can take between q_a and q_b.

Let us work out the above considerations in a more precise way.[9] We are interested in the amplitude for a particle which is in a position eigenstate $|q_a\rangle$ at time t_a to be found in a position eigenstate $|q_b\rangle$ at a later time t_b.[10] The amplitude is given by

$$G = \langle q_b|\, \hat{U}(t_b, t_a)\, |q_a\rangle$$

where

$$\hat{U}(t_b, t_a) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t_b - t_a)}$$

is the unitary time-evolution operator for a time-independent Hamiltonian $\hat{H}$. (The initial state is $|q_a\rangle$; we then time-evolve the system from t_a to t_b, and ask what the overlap with a position eigenstate $|q_b\rangle$ is.)

To calculate G, we split the time interval $t_b - t_a$ into N subintervals of size $\Delta t = (t_b - t_a)/N$. From quantum mechanics, we know that

$$\hat{U}(t_b, t_a) = \hat{U}(t_b, t_x)\hat{U}(t_x, t_a)\,, \quad t_b > t_x > t_a$$

and the propagator G becomes

$$G = \langle q_b| \left(\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t}\right)^N |q_a\rangle = \langle q_b|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \cdots \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t}\, |q_a\rangle$$

In this way, we can consider the evolution of the particle from q_a to q_b as the limiting process of a discrete evolution between position q_n at time $t_a + n\Delta t$ and q_{n+1} at time $t_a + (n+1)\Delta t$ obtained by application of the operator

$$U(t_a + (n+1)\Delta t, t_a + n\Delta t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t}\,.$$

[9] The formalism used here was invented before Feynman, namely by Dirac.

[10] Here we assume $t_b > t_a$. Alternatively, the propagator is often defined with an additional $\theta(t_b - t_a)$ to ensure causality.

To proceed with our calculation of G, we will insert $N-1$ complete sets of position eigenstates with $\int \mathrm{d}q_n \, |q_n\rangle \langle q_n| = 1$ to obtain

$$\begin{aligned} G = \langle q_b| \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \underbrace{\int \mathrm{d}q_{N-1} \, |q_{N-1}\rangle \langle q_{N-1}|}_{1} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \underbrace{\int \mathrm{d}q_{N-2} \, |q_{N-2}\rangle \langle q_{N-2}|}_{1} \cdots \\ \cdots \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \underbrace{\int \mathrm{d}q_{n+1} \, |q_{n+1}\rangle \langle q_{n+1}|}_{1} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \underbrace{\int \mathrm{d}q_n \, |q_n\rangle \langle q_n|}_{1} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \cdots \\ \cdots \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \underbrace{\int \mathrm{d}q_2 \, |q_2\rangle \langle q_2|}_{1} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \underbrace{\int \mathrm{d}q_1 \, |q_1\rangle \langle q_1|}_{1} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \, |q_a\rangle \end{aligned}$$

which we can rewrite as

$$G = \int \mathrm{d}q_1 \cdots \mathrm{d}q_{N-1} \, \langle q_b| \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \, |q_{N-1}\rangle \cdots \langle q_{n+1}| \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \, |q_n\rangle \cdots \langle q_1| \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \, |q_a\rangle$$

Here, we have a product of N terms G_n, but only integrate over $N-1$ variables q_n. This form resembles our sum over products of amplitudes in the introduction. We proceed by considering the propagator between time slices n and $n+1$,

$$G_n = \langle q_{n+1}| \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} \, |q_n\rangle$$

To evaluate this expression, we assume a Hamiltonian

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

make the Suzuki-Trotter approximation[11]

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\Delta t} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{\hat{p}^2}{2m}\Delta t} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{V}\Delta t} + \mathcal{O}(\Delta t^2)$$

and insert a complete set of momentum eigenstates:

$$\begin{aligned} G_n &\simeq \int \mathrm{d}p \, \langle q_{n+1}| \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{\hat{p}^2}{2m}\Delta t} \, |p\rangle \langle p| \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{V}(\hat{q})\Delta t} \, |q_n\rangle \\ &= \int \mathrm{d}p \, \langle q_{n+1} \, | \, p\rangle \langle p \, | \, q_n\rangle \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}\Delta t} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(q_n)\Delta t} \end{aligned}$$

[11] We use the Baker-Campbell-Hausdorff formula

$$\mathrm{e}^{\epsilon(A+B)} = \mathrm{e}^{\epsilon A} \mathrm{e}^{\epsilon B} \mathrm{e}^{\epsilon^2 C} \, , \quad C = \tfrac{1}{2}[A,B] + \mathcal{O}(\epsilon)$$

The inner products of position and momentum eigenstates are known from quantum mechanics (cf. the Fourier transformation in chapter 1):

$$\langle q \,|\, p \rangle = \langle p \,|\, q \rangle^* = \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{\mathrm{i}pq}$$

Therefore, we can write

$$G_n \simeq \int \frac{\mathrm{d}p}{2\pi\hbar} \mathrm{e}^{\mathrm{i}q_{n+1}p} \mathrm{e}^{-\mathrm{i}q_n p} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}\Delta t} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(q_n)\Delta t} = \frac{1}{2\pi\hbar} \int \mathrm{d}p \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}\Delta t + \mathrm{i}p(q_{n+1}-q_n)} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(q_n)\Delta t}$$

which does not contain any more operators. The integral over p is of the Gaussian type, and can be carried out using

$$\int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-ax^2/2+bx} = \sqrt{\frac{2\pi}{a}} \mathrm{e}^{b^2/2a}$$

to obtain ($a = \mathrm{i}\Delta t/(\hbar m)$, $b = \mathrm{i}(q_{n+1} - q)/\hbar$)

$$\begin{aligned} G_n &\simeq \frac{1}{2\pi} \left(\frac{2\pi\hbar m}{\mathrm{i}\Delta t} \right)^{\frac{1}{2}} \mathrm{e}^{-(q_{n+1}-q)^2/(2\mathrm{i}\Delta t/m)} \mathrm{e}^{-\mathrm{i}V(q_n)\Delta t} \\ &= \left(\frac{-\mathrm{i}m}{2\pi\hbar\Delta t} \right)^{\frac{1}{2}} \mathrm{e}^{\frac{\mathrm{i}m}{2\hbar}\frac{(q_{n+1}-q_n)^2}{\Delta t^2}\Delta t} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(q_n)\Delta t} \end{aligned}$$

The total propagator then takes the form[12]

$$\begin{aligned} G &\simeq \frac{1}{\xi} \prod_{n=1}^{N-1} \int \frac{\mathrm{d}q_n}{\xi} \mathrm{e}^{\frac{\mathrm{i}m}{2\hbar}\frac{(q_{n+1}-q_n)^2}{\Delta t^2}\Delta t} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V(q_n)\Delta t}, \quad \xi = \left(\frac{-\mathrm{i}m}{2\pi\hbar\Delta t} \right)^{-\frac{1}{2}} \\ &= \frac{1}{\xi} \left[\prod_{n=1}^{N-1} \int \frac{\mathrm{d}q_n}{\xi} \right] \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Delta t \sum_n \left[\frac{m}{2}\frac{(q_{n+1}-q_n)^2}{\Delta t^2} - V(q_n) \right]}. \end{aligned}$$

The $\simeq$ sign in the first line is due to the Trotter approximation.

Strong fluctuations of the path on small length scales are suppressed by the factor $(q_{n+1} - q_n)^2$ (the resulting large phase fluctuations gives rise to a cancellation of the contributions of such paths to the total amplitude). This suggests to consider the limit $N \to \infty$, $\Delta t \to 0$ with $N\Delta t = \text{const.}$, in which

$$\sum_n \Delta t \to \int \mathrm{d}t\,, \quad \frac{(q_{n+1} - q_n)^2}{\Delta t^2} \to \dot{q}^2\,, \quad \left[\prod_{n=1}^{N-1} \int \frac{\mathrm{d}q_n}{\xi} \right] \to \int \mathcal{D}[q(t)]$$

[12] We have one ξ^{-1} for each of the N integrated momenta.

and

$$G = \int \mathcal{D}[q(t)] \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\left[\frac{m}{2}\dot{q}^2 - V(q)\right]} = \int \mathcal{D}[q(t)] \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t L} = \int \mathcal{D}[q(t)] \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S} \,.$$

(In the limit $\Delta t \to 0$, the Suzuki-Trotter approximation becomes exact.)

The above result implies that a quantum mechanical amplitude is given by the sum/integral over all possible paths that connect the initial and final state. Remarkably, all paths have the same weight $|\mathrm{e}^{\mathrm{i}S/\hbar}| = 1$. The special role of the classical path emerges from the cancellation of the contributions from paths that have very different phases. We can define a coherent interval around the classical path by the condition that $(S - S')/\hbar \lesssim \pi$. The amplitudes of such paths combine constructively so that the particle has a high probability to be observed along them. In contrast, for paths outside this range, the phase difference is essentially random and destructive interference sets in. The classical path is special because the action is stationary and does not change (to first order) upon variations of the path. In the classical limit $\hbar \to 0$, any variation of the path leads to an infinite phase so that only the classical path remains.

3.2 More general cases and gory details

While the above derivation was intuitive, we glossed over some important details, and had to assume an explicit simple form for the kinetic energy. Let us also consider a more general Hamiltonian $\hat{H} = \hat{T} + \hat{V}$. In this case, we obtain for the amplitude

$$G \simeq \left[\prod_{n=1}^{N-1} \int \mathrm{d}q_n\right] \left[\prod_{n=1}^{N} \int \frac{\mathrm{d}p_n}{2\pi\hbar}\right] \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{\hbar}\sum_{n=0}^{N-1}\left(V(q_n) + T(p_{n+1}) - p_{n+1}\frac{q_{n+1}-q_n}{\Delta t}\right)}$$

with the conditions $q_0 = q_a$, $q_N = q_b$.[13] This form of the propagator indicates that at each time slice, we integrate over the classical phase space (q_n, p_n).

[13] Note that for N time slices, we have N integrals over momenta but only $N-1$ integrals over position. The reason is that we only insert $N-1$ sets of position eigenstates since we get $\langle q_b| = \langle q_N|$ and $|q_a\rangle = |q_0\rangle$ from the definition of the amplitude itself.

The continuum limit amounts to

$$\sum_{n=0}^{N-1} \Delta t \to \int_{t_a}^{t_b} \mathrm{d}t\,, \quad \frac{(q_{n+1}-q_n)}{\Delta t} \to \dot{q}_{t=t_n}\,,$$

as well as

$$V(q_n) + T(p_{n+1}) \to T(p|_{t=t_n}) + V(q|_{t=t_n}) = H(p|_{t=t_n}, q|_{t=t_n})$$

and the definition of a new measure

$$\lim_{N\to\infty} \left[\prod_{n=1}^{N-1} \int \mathrm{d}q_n\right] \left[\prod_{n=1}^{N} \int \frac{\mathrm{d}p_n}{2\pi\hbar}\right] \equiv \int_{\substack{q(t_b)=q_b \\ q(t_a)=q_a}} \mathcal{D}[q]$$

The propagator takes the form

$$G = \int_{\substack{q(t_b)=q_b \\ q(t_a)=q_a}} \mathcal{D}[q] \exp\left[\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t(p\dot{q} - H(p,q))\right]$$

If the kinetic energy is quadratic in the momenta, the corresponding integrals are Gaussian and can be carried out to find

$$\begin{aligned} G &= \int_{\substack{q(t_b)=q_b \\ q(t_a)=q_a}} \mathcal{D}[q] \exp\left[-\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t V(q)\right] \int \mathcal{D}[p] \exp\left[-\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t \left(\frac{p^2}{2m} - p\dot{q}\right)\right] \\ &= \int_{\substack{q(t_b)=q_b \\ q(t_a)=q_a}} \mathcal{D}[q] \exp\left[\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t L(q,\dot{q})\right]\,, \end{aligned}$$

with the Lagrangian

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

and the integration measure

$$\mathcal{D}[q] = \lim_{N\to\infty} \left(\frac{Nm}{\mathrm{i}(t_b-t_a)2\pi\hbar}\right)^{\frac{N}{2}} \prod_{n=1}^{N-1} \mathrm{d}q_n$$

- While providing a more satisfactory notation in terms of derivatives, it is highly nontrivial to ensure that the continuous path integral is well defined mathematically. For calculations and simulations, one therefore often resorts to the discrete definition.

- In the limit $N \to \infty$, the path integral becomes infinite dimensional. In particular, we integrate over all possible functions $q(t)$ with boundary conditions $q(t_a) = q_a$, $q(t_b) = q_b$. An integral for which the domain of integration is a space of functions is called a functional integral.

3.3 Relation to the wave function

The path integral offers an alternative approach to quantum mechanics in which the wave function (at first sight) does not enter the picture. However, since the two approaches are completely equivalent, let us make the connection a bit more clear.

First, a more general amplitude between an initial state $|\psi_a\rangle$ at $t = t_a$ and a final state $|\psi_b\rangle$ at time $t = t_b$ is obtained from

$$\langle \psi_b | \, \mathrm{e}^{-\mathrm{i}\hat{H}(t_b - t_a)} \, |\psi_a\rangle = \int \mathrm{d}q_a \int \mathrm{d}q_b \underbrace{\langle \psi_b \mid q_b \rangle}_{\psi_b^*(q_b)} \langle q_b | \, \mathrm{e}^{-\mathrm{i}\hat{H}(t_b - t_a)} \, |q_a\rangle \underbrace{\langle q_a \mid \psi_a \rangle}_{\psi_a(q_a)} .$$

In particular, the amplitude

$$\langle q, t \mid \psi \rangle = \langle q | \, \mathrm{e}^{-\mathrm{i}\hat{H}t} \, |\psi\rangle = \int \mathrm{d}q_a \, \langle q | \, \mathrm{e}^{-\mathrm{i}\hat{H}t} \, |q_a\rangle \, \langle q_a \mid \psi \rangle$$

is nothing but the wave function $\psi(q, t)$ that gives the amplitude for the particle to be found at q, t. Hence, the wave function is the propagator integrated over all possible initial states q_a, and contains less information (it does not specify where the particle came from).

If we know the eigenstates of $\hat{H}$, we can write

$$\begin{aligned} \langle q_b | \, \mathrm{e}^{-\mathrm{i}\hat{H}(t_b - t_a)} \, |q_a\rangle &= \sum_n \langle q_b | \, \mathrm{e}^{-\mathrm{i}\hat{H}(t_b - t_a)} \, |n\rangle \, \langle n \mid q_a \rangle \\ &= \sum_n \langle q_b \mid n \rangle \, \langle n \mid q_a \rangle \, \mathrm{e}^{-\mathrm{i}E_n(t_b - t_a)} \\ &= \sum_n \phi_n(q_b) \phi_n^*(q_a) \mathrm{e}^{-\mathrm{i}E_n(t_b - t_a)} . \end{aligned}$$

3.4 Gaussian integration

Before we calculate path integrals, we need to brush up our knowledge about Gaussian integrals. We do so in a series of steps, starting with

$$\int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-x^2} = \sqrt{\pi}$$

The first generalization is the replacement $x \to x\sqrt{a/2}$, which gives

$$\int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-ax^2/2} = \sqrt{\frac{2\pi}{a}}$$

We can also add a linear term in the exponent,

$$\int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-ax^2/2+bx} = \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-\frac{a}{2}\left(x-\frac{b}{a}\right)^2} \mathrm{e}^{\frac{b^2}{2a}} = \mathrm{e}^{\frac{b^2}{2a}} \int_{-\infty}^{\infty} \mathrm{d}y \mathrm{e}^{-\frac{a}{2}y} = \sqrt{\frac{2\pi}{a}} \mathrm{e}^{\frac{b^2}{2a}}$$

A useful trick to complete the square is as follows. The function $Q(x) = (x-\beta)^2$ has a minimum or maximum at $x = x_0 = \beta$ where $Q(x_0) = 0$, as reflected in the derivative $Q'(x) = 2x - 2\beta$. Given a function $P(x) = x^2 - 2\beta x$, we see that $P'(x) = Q'(x)$, and $P(x)$ also has a minimum or maximum $P(x_0)$ at $x_0 = \beta$. To rewrite $P(x)$ in the form $(x-\beta)^2$, we simply consider $P(x) - P(x_0)$ which vanishes at $x = x_0$. Of course, we have to subtract and add $P(x_0)$ to keep the result invariant. In the above example, we have $P(x) = -ax^2/2 + bx = -\frac{a}{2}(x^2 - \frac{2b}{a}x)$ and hence

$$P'(x) = -\frac{a}{2}\left(2x - \frac{2b}{a}\right) \stackrel{!}{=} 0 \;\leftrightarrow\; x_0 = \frac{b}{a}\,, \quad P(x_0) = \frac{b^2}{2a}$$

We therefore consider

$$\begin{aligned} P(x) - P(x_0) + P(x_0) &= -\frac{a}{2}\left(x^2 - \frac{2b}{a}x\right) - \frac{b^2}{2a} + \frac{b^2}{2a} \\ &= -\frac{a}{2}\left(x - \frac{b}{a}\right)^2 + \frac{b^2}{2a} \end{aligned}$$

In anticipation of later results, it is useful to rewrite our above result as

$$\int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-x\frac{a}{2}x+bx} = \sqrt{\frac{2\pi}{a}} \mathrm{e}^{\frac{1}{2}b\frac{1}{a}b}$$

Note that we have *integrated out* x, which does not appear on the r.h.s.

The next step is to replace the variable x by an N-component vector $\vec{x}$, which could represent the discrete approximation of a field. Accordingly, we replace a by a matrix A and consider

$$\int_{-\infty}^{\infty} \mathrm{d}x_1 \mathrm{d}x_2 \cdots \mathrm{d}x_N \mathrm{e}^{-\frac{1}{2}\sum_{ij} x_i A_{ij} x_j} = \int_{-\infty}^{\infty} \mathrm{d}\vec{x}\, \mathrm{e}^{-\frac{1}{2}\vec{x}^T A\, \vec{x}}$$

Assuming A to be real and symmetric, we can transform into a basis where it is diagonal: $A \mapsto O^T D O$ with $D = \mathrm{diag}(D_{11}, D_{22}, \cdots, D_{NN})$. Inserting this transformation and changing the integration variables to $\vec{y} = O\vec{x}$ (orthogonal transformation, so the Jacobian is one) we get

$$\int_{-\infty}^{\infty} \mathrm{d}\vec{x}\, \mathrm{e}^{-\frac{1}{2}\vec{x}^T O^T A\, O\vec{x}} = \int_{-\infty}^{\infty} \mathrm{d}\vec{y}\, \mathrm{e}^{-\frac{1}{2}\vec{y}^T D\, \vec{y}} = \int_{-\infty}^{\infty} \mathrm{d}\vec{y}\, \mathrm{e}^{-\frac{1}{2}\sum_i y_i D_{ii} y_i}$$

In the diagonal basis, we can factorize the integral into N integrals that we know how to solve:

$$\prod_{i=1}^{N} \int_{-\infty}^{\infty} \mathrm{d}y_i\, \mathrm{e}^{-\frac{1}{2}D_{ii}y_i^2} = \prod_{i=1}^{N} \sqrt{\frac{2\pi}{D_{ii}}} = \frac{(2\pi)^{N/2}}{(D_{11}\cdots D_{NN})^{1/2}} = \frac{(2\pi)^{N/2}}{(\det D)^{1/2}} = \sqrt{\frac{(2\pi)^N}{\det A}}$$

so that we have

$$\int_{-\infty}^{\infty} \mathrm{d}\vec{x}\, \mathrm{e}^{-\frac{1}{2}\vec{x}^T A\, \vec{x}} = \sqrt{\frac{(2\pi)^N}{\det A}} \tag{3}$$

We can again extend this to include a linear term:

$$\boxed{\int \mathrm{d}\vec{x}\, \mathrm{e}^{-\frac{1}{2}\vec{x}^T A\vec{x} + \vec{b}^T\vec{x}} = \sqrt{\frac{(2\pi)^N}{\det A}} \mathrm{e}^{\frac{1}{2}\vec{b}^T A^{-1}\vec{b}}}$$

The generalization to complex vectors is

$$\int \mathrm{d}(\vec{z}^\dagger, \vec{z})\, \mathrm{e}^{-\frac{1}{2}\vec{z}^\dagger A\vec{z} + \vec{w}^\dagger\vec{z} + \vec{z}^\dagger\vec{w}'} = \pi^N \det A^{-1} \mathrm{e}^{\frac{1}{2}\vec{w}^\dagger A^{-1}\vec{w}'}$$

where $\mathrm{d}(\vec{z}^\dagger, \vec{z}) = \prod_{i=1}^{N} \mathrm{dRe}\, z_i \mathrm{dIm}\, z_i$ and $\vec{z}^\dagger$ is the transpose and complex conjugate of $\vec{z}$.

Finally, especially for the functional integral, we will consider the limit $N \to \infty$, where the vectors turn into functions ($\vec{x} \mapsto f(x)$, a scalar field) and the

matrix A will correspond to a differential operator ($A_{ij} \mapsto A(x,y)$). Using the discrete representation and then taking the limit gives in the real case

$$\int \mathcal{D}[f]\, \mathrm{e}^{-\frac{1}{2}\iint \mathrm{d}x\mathrm{d}y\, f(x)A(x,y)f(y)+\int \mathrm{d}x\, b(x)f(x)} = \frac{B}{\sqrt{\det A(x,y)}} \mathrm{e}^{\frac{1}{2}\iint \mathrm{d}x\mathrm{d}y\, b(x)A^{-1}(x,y)b(y)}$$

or written in a more compact way

$$\boxed{\int \mathcal{D}[f]\, \mathrm{e}^{-\frac{1}{2}\iint fAf+\int bf} = N\mathrm{e}^{\frac{1}{2}\iint bA^{-1}b}} \tag{4}$$

- B is essentially $(2\pi)^{\infty}$. Typically, the prefactor will drop out when we calculate observables, or we can use known limiting cases of the propagator to regularize the answer.
- $A^{-1}(x,y) = G(x,y)$ is the Green function of the differential operator $A(x,y) = \hat{A}$, which is defined via

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

  and provides a solution of an inhomogeneous linear differential equation $\hat{L}_x u(x) = J(x)$ in the form

  $$u(x) = \int \mathrm{d}x' G(x,x')J(x')$$

  For example, the propagator $G(x,t_x,y,t_y) = \langle x|\, \hat{U}(t_x,t_y)\, |y\rangle$ is the Green function of the time-dependent Schrödinger equation.

3.5 Propagator of the free particle

We begin with an approximate treatment (something we will introduce as the stationary phase approximation or the semiclassical limit later) that turns out to give the correct result for a free particle. It is based on the idea that the path integral is dominated by the contributions of paths close to the classical solution q_{cl}. Because S stationary, we assume that all these paths

contribute the same factor $\mathrm{e}^{\mathrm{i}S_{\mathrm{cl}}/\hbar}$ and that the number of relevant paths gives an overall prefactor so that

$$G(t_b, q_b, t_a, q_a) \sim A' \mathrm{e}^{\mathrm{i}S_{\mathrm{cl}}/\hbar} .$$

The classical path is given by

$$q_{\mathrm{cl}}(t) = q_a + \frac{q_b - q_a}{t_b - t_a}(t - t_a) \tag{5}$$

and leads to the action

$$S_{\mathrm{cl}} = \int_{t_a}^{t_b} \frac{m}{2} \left(\frac{q_b - q_a}{t_b - t_a} \right)^2 = \frac{m}{2} \frac{(q_b - q_a)^2}{t_b - t_a}$$

Therefore, we have for the propagator

$$G(t_b, q_b, t_a, q_a) = A' \exp \left[\frac{\mathrm{i}m(q_b - q_a)^2}{2\hbar(t_b - t_a)} \right]$$

The prefactor A' is determined by the condition that

$$\lim_{t \to t'} G(t, q, t', q') = \langle q \,|\, q' \rangle = \delta(q - q') .$$

Representing the Dirac δ function as the limit of a Gaussian distribution,

$$\delta(x - x') = \lim_{\epsilon \to 0} \frac{1}{\sqrt{\pi \epsilon^2}} \mathrm{e}^{-\frac{(x-x)^2}{\epsilon^2}} ,$$

we have

$$\epsilon^2 = \frac{2\mathrm{i}\hbar}{m}(t_b - t_a) , \quad A' = \frac{1}{\sqrt{\pi \epsilon^2}} = \sqrt{\frac{m}{2\pi \mathrm{i}\hbar(t_b - t_a)}}$$

and find the propagator

$$G(t_b, q_b, t_a, q_a) = \sqrt{\frac{m}{2\pi \mathrm{i}\hbar(t_b - t_a)}} \exp \left[\frac{\mathrm{i}m(q_b - q_a)^2}{2\hbar(t_b - t_a)} \right] .$$

The exponential part is the contribution from the classical path given by equation (5), while the prefactor accounts for the effect of quantum fluctuations.

We can confirm this result using the discrete definition of the path integral. For a free particle, the action is

$$S = \sum_{i=0}^{N-1} \frac{m}{2} \left(\frac{q_{i+1} - q_i}{\Delta t} \right)^2 \Delta t$$

and the propagator takes the form (we assume that we do not know the measure exactly, hence the factor A)

$$\begin{aligned} G(t_b, q_b, t_a, q_a) &= \int \mathcal{D}[q(t)] \mathrm{e}^{\mathrm{i}S/\hbar} \\ &= \lim_{\substack{N\to\infty \\ \Delta t\to 0}} A \int_{-\infty}^{\infty} \mathrm{d}q_1 \cdots \mathrm{d}q_{N-1} \exp\left[\frac{\mathrm{i}}{\hbar} \sum_{i=0}^{N-1} \frac{m}{2} \left(\frac{q_{i+1} - q_i}{\Delta t} \right)^2 \Delta t \right]_{\substack{q_0 = q_a \\ q_N = q_b}} \end{aligned}$$

We first transform to variables

$$y_i = \left(\frac{m}{2\hbar \Delta t} \right)^{1/2} q_i$$

to obtain

$$G(t_b, q_b, t_a, q_a) = \lim_{\substack{N\to\infty \\ \Delta t\to 0}} A \left(\frac{2\hbar \Delta t}{m} \right)^{\frac{N-1}{2}} \int_{-\infty}^{\infty} \mathrm{d}y_1 \cdots \mathrm{d}y_{N-1} \exp\left[\sum_{i=0}^{N-1} \frac{(y_{i+1} - y_i)^2}{\mathrm{i}} \right]$$

Let us start with the integral over y_1:

$$I_1 = \int \mathrm{d}y_1 \exp\left[-\frac{1}{\mathrm{i}} (y_1 - y_0)^2 - \frac{1}{\mathrm{i}} (y_2 - y_1)^2 \right] = \sqrt{\frac{\mathrm{i}\pi}{2}} \exp\left[-\frac{1}{2\mathrm{i}} (y_2 - y_0)^2 \right]$$

Integrating over the next time slice (i.e., y_2) amounts to

$$\begin{aligned} I_2 &= \sqrt{\frac{\mathrm{i}\pi}{2}} \int \mathrm{d}y_2 \exp\left[-\frac{1}{\mathrm{i}} (y_3 - y_2)^2 - \frac{1}{2\mathrm{i}} (y_2 - y_0)^2 \right] \\ &= \sqrt{\frac{\mathrm{i}\pi}{2}} \sqrt{\frac{2\mathrm{i}\pi}{3}} \exp\left[-\frac{1}{3\mathrm{i}} (y_3 - y_0)^2 \right] \\ &= \left(\frac{(\mathrm{i}\pi)^2}{3} \right)^{1/2} \exp\left[-\frac{1}{3\mathrm{i}} (y_3 - y_0)^2 \right] \end{aligned}$$

Integrating over all the $N-1$ variables y_i gives the result

$$I_{N-1} = \frac{(\mathrm{i}\pi)^{(N-1)/2}}{N^{1/2}} \exp\left[-\frac{1}{N\mathrm{i}}(y_N - y_0)^2\right]$$

Switching back to the original variables q_i, the propagator takes the form

$$G = \lim_{\substack{N\to\infty \\ \Delta t\to 0}} A \left(\frac{2\hbar\Delta t}{m}\right)^{\frac{N-1}{2}} \frac{(\mathrm{i}\pi)^{(N-1)/2}}{N^{1/2}} \exp\left[-\frac{m}{2\hbar\Delta t N\mathrm{i}}(q_N - q_0)^2\right]$$

Since we know the exact result for $N \to \infty$ from above, we write this as

$$G = \lim_{\substack{N\to\infty \\ \Delta t\to 0}} A \left(\frac{2\mathrm{i}\pi\hbar\Delta t}{m}\right)^{\frac{N}{2}} \left(\frac{m}{2\pi\mathrm{i}\hbar N\Delta t}\right)^{\frac{1}{2}} \exp\left[-\frac{m}{2\hbar\Delta t N\mathrm{i}}(q_N - q_0)^2\right]$$

In the continuum limit, $N\Delta t \to (t_b - t_a)$, and in order to reproduce the result from above, we need

$$\lim_{\substack{N\to\infty \\ \Delta t\to 0}} A \left(\frac{2\mathrm{i}\pi\hbar\Delta t}{m}\right)^{\frac{N}{2}} = 1$$

which implies that (we found the same ξ in the derivation of the path integral)

$$A = \left(\frac{2\mathrm{i}\pi\hbar\Delta t}{m}\right)^{-N/2} = \xi^{-N}, \quad \xi = \left(\frac{2\mathrm{i}\pi\hbar\Delta t}{m}\right)^{1/2}$$

A hence cancels the formally divergent prefactor, and we obtain the integration measure for the continuous path integral of the free particle:

$$\int \mathcal{D}[q(t)] = \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \frac{1}{\xi} \int_{-\infty}^{\infty} \int \cdots \int_{-\infty}^{\infty} \frac{\mathrm{d}q_1}{\xi} \frac{\mathrm{d}q_1}{\xi} \cdots \frac{\mathrm{d}q_{N-1}}{\xi},$$

which will also be useful for more complicated problems.

Let us consider the propagator as a function of $q = q_b - q_a$ at a fixed time T,

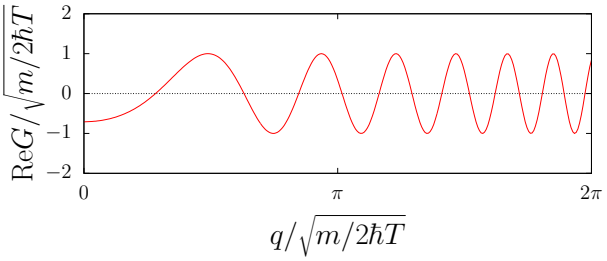
$$G(T, q, 0, 0) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar T}} \exp\left[\frac{\mathrm{i}mq^2}{2\hbar T}\right],$$

which oscillates with a frequency that increases with increasing q. For sufficiently large q, the frequency is approximately constant over several periods, and we can consider the wavelength λ:

$$2\pi = \frac{m(q+\lambda)^2}{2\hbar T} - \frac{mq^2}{2\hbar T} \approx \frac{mq\lambda}{\hbar T}$$

Classically, a free particle travelling from 0 to q in time T has a velocity q/T and a momentum $p = mq/T$. If the quantum particle can be considered to have momentum p, the amplitude oscillates with the de Broglie wavelength:

$$\lambda = 2\pi\frac{\hbar T}{mq} = \frac{h}{p}\,.$$



3.6 Propagator of the harmonic oscillator

As another example, let us calculate the path integral for the quantum harmonic oscillator. To be concrete, we will calculate the amplitude for the oscillator to have coordinate $q_a = 0$ at $t_a = 0$, and $q_b = 0$ at $t_b = T$, given by

$$\begin{aligned} G(q_b = 0, t_b = T, q_a = 0, t_a = 0) &= \langle q_b = 0, t_b = T \mid q_a = 0, t_a = 0\rangle \\ &= \int_{q_a=0,t=0}^{q_b=0,t=T} \mathcal{D}[q(t)]\mathrm{e}^{\mathrm{i}\int_0^T \mathrm{d}t L[q(t),\dot{q}(t)]} \end{aligned}$$

The classical Lagrangian has the form (cf. the Hamiltonian on p. 12)

$$L = \frac{m\dot{q}^2}{2} - \frac{m\omega_0^2 q^2}{2}$$

so that we have to calculate

$$G(0,T,0,0) = \int_{q_a=0,t=0}^{q_b=0,t=T} \mathcal{D}[q(t)]\mathrm{e}^{\frac{\mathrm{i}m}{2}\int_0^T \mathrm{d}t(\dot{q}^2-\omega_0^2 q^2)}\,.$$

To cast the integral into the form of a Gaussian integral, we integrate by parts and exploit that fact that we want $q = 0$ at $t = 0$ and $t = T$:

$$S = \frac{m}{2}\int_0^T \mathrm{d}t\left[\left(\frac{\mathrm{d}q}{\mathrm{d}t}\right)^2 - \omega_0^2 q^2\right] = \frac{m}{2}\left\{q(t)\dot{q}(t)|_0^T - \int_0^T \mathrm{d}t q(t)\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} - \int_0^T \mathrm{d}t\omega_0^2 q^2\right\}$$

which allows us to rewrite the amplitude as

$$G = \int \mathcal{D}[q(t)] \mathrm{e}^{\frac{\mathrm{i}m}{2}\int_0^T \mathrm{d}t q(t)(-\partial_t^2-\omega_0^2)q(t)} = \int \mathcal{D}[q(t)] \mathrm{e}^{-\frac{1}{2}\int_0^T \mathrm{d}t q(t)\hat{A}q(t)} \,.$$

The integral now has the form of equation (4), with $b = 0$ and $\hat{A} = -\mathrm{i}m(-\partial_t^2 - \omega_0^2)$ (since our oscillator has no spatial dimension, we only have a time coordinate). While we can always return to the discrete case to evaluate the path integral, let us proceed differently here. The exponent takes the form

$$-\tfrac{1}{2}\int_0^T \mathrm{d}t q(t)\hat{A}q(t) = \frac{\mathrm{i}}{2}\int_0^T \mathrm{d}t\, q(t)[-m\partial_t^2 - m\omega_0^2]\, q(t)$$

where the functions $q(t)$ have the boundary conditions $q(0) = q(T) = 0$. Let $\{\psi_n(t)\}$ be a complete set of eigenfunctions (solutions) of $\hat{A}$, with

$$\begin{aligned} \hat{A}\psi_n &= A_n\psi_n \,, \\ \psi_n(0) &= \psi_n(T) = 0 \,, \\ \sum_n \psi_n^*(t)\psi_n(t') &= \delta(t-t') \,, \\ \int_0^T \mathrm{d}t\, \psi_n^*(t)\psi_m(t) &= \delta_{nm} \,. \end{aligned}$$

We can expand the paths $q(t)$ with $q(0) = q(T) = 0$ in this basis:

$$q(t) = \sum_n c_n\psi_n(t) \,.$$

For the harmonic oscillator, the eigenfunctions take the form

$$\psi_n(t) = b_n \sin(\omega_n t)$$

with frequencies

$$\omega_n = \frac{n\pi}{T} \,, \quad n = 1, 2, \ldots$$

The eigenvalues of $\hat{A}$ are obtained from

$$\hat{A}\psi_n = -\mathrm{i}m(-\partial_t^2 - \omega_0^2)b_n \sin(\omega_n t) = -\mathrm{i}m(\omega_n^2 - \omega_0^2)b_n \sin(\omega_n t) = A_n\psi_n(t).$$

The exponent in the integral can be written as

$$-\tfrac{1}{2}\int_0^T \mathrm{d}t q(t)\hat{A}q(t) = -\tfrac{1}{2}\int_0^T \mathrm{d}t \sum_m c_m\psi_m(t)\hat{A}\sum_n c_n\psi_n(t) = -\tfrac{1}{2}\sum_n c_n^2 A_n$$

and the path integral can be written in terms of an integral over the coefficients c_n (the transformation $q(t) \to c_n$ is canonical, and the integral over all c_n gives us all possible paths):

$$\int \mathcal{D}[q(t)] \mapsto B \prod_n \int \frac{\mathrm{d}c_n}{\sqrt{2\pi}}$$

where B is a constant to be determined below. We now have a product of Gaussian integrals[14] that we can evaluate to obtain

$$G = B \int \left[\prod_n \frac{\mathrm{d}c_n}{\sqrt{2\pi}} \right] \mathrm{e}^{-\frac{1}{2}\sum_n c_n^2 A_n} = B \prod_n \frac{1}{\sqrt{2\pi}} \sqrt{\frac{2\pi}{A_n}} = B \frac{1}{\sqrt{\prod_n A_n}}$$

It is customary to define the determinant of the operator $\hat{A}$ as the product of its eigenvalues A_n,

$$\prod_n A_n \equiv \det \hat{A} \,.$$

Inserting the definition of ω_n and absorbing $i^{N/2}$ in the prefactor, we have

$$G(0,T,0,0) = B' \left\{ \prod_{n=1}^{\infty} m \left[\left(\frac{n\pi}{T} \right)^2 - \omega_0^2 \right] \right\}^{-1/2}$$

The product is formally divergent, but will be regularized by the prefactor B'. To obtain the physical answer, we exploit the fact that we know the corresponding propagator for a free particle

$$G_0(0,T,0,0) = \left(\frac{-\mathrm{i}m}{2\pi T} \right)^{1/2}$$

and that the latter has to coincide with $G(0,T,0,0)$ above for $\omega_0 = 0$ (i.e., $V = 0$), that is $G_0/G_{\omega_0=0} = 1$. Multiplying with $G_0/G_{\omega_0=0}$ gives

$$\begin{aligned} G(0,T,0,0) &= G(0,T,0,0) \frac{G_0}{G_{\omega_0=0}} \\ &= \frac{B' \left\{ \prod_{n=1}^{\infty} m \left[\left(\frac{n\pi}{T} \right)^2 - \omega_0^2 \right] \right\}^{-1/2}}{B' \left\{ \prod_{n=1}^{\infty} m \left[\left(\frac{n\pi}{T} \right)^2 \right] \right\}^{-1/2}} \left(\frac{-\mathrm{i}m}{2\pi T} \right)^{1/2} \end{aligned}$$

[14] We have a discrete product but have avoided a discretization of time.

and hence the well-defined expression

$$G(0,T,0,0) = \left\{ \prod_{n=1}^{\infty} \left[1 - \left(\frac{\omega_0 T}{n\pi} \right)^2 \right] \right\}^{-1/2} \left(\frac{-\mathrm{i}m}{2\pi T} \right)^{1/2}$$

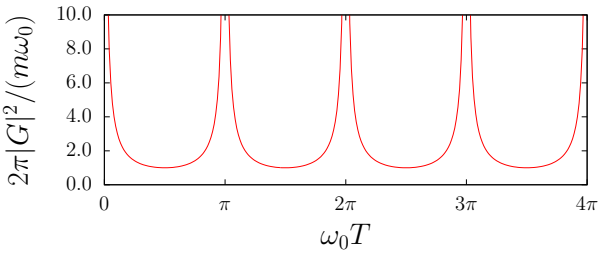
In a final step, we can use the identity

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

to write the propagator as (we add $\hbar$ at the end)

$$G(0,T,0,0) = \left(\frac{-\mathrm{i}m\omega_0}{2\pi\hbar \sin \omega_0 T} \right)^{\frac{1}{2}}$$

from which we can obtain the probability density $|G|^2$ shown below. Classically, the oscillator starts at $q = 0$ and returns to the initial position at times $T = n\omega_0/\pi$ (i.e., twice per period). Quantum mechanically, paths which begin and end at $q = 0$ in time T interfere constructively if $T = n\omega_0/\pi$, whereas for other times some random phase cancellation takes place. Note that the probability for the oscillator to be $q = 0$ remains nonzero at all times.



A similar (but more involved) calculation gives the propagator for general initial/final times and positions,

$$G(q_b,t_b,q_a,t_a) = \left(\frac{-\mathrm{i}m\omega_0}{2\pi\hbar \sin[\omega_0(t_b-t_a)]} \right)^{\frac{1}{2}} \mathrm{e}^{\mathrm{i}S_{\mathrm{cl}}/\hbar} \tag{6}$$

$$S_{\mathrm{cl}} = \tfrac{1}{2} m\omega_0 \csc[\omega_0(t_b-t_a)] \left\{ (q_a^2+q_b^2)\cos[\omega_0(t_b-t_a)] - 2q_aq_b \right\} .$$

3.7 Newton's law, commutators, Brownian motion

The path-integral approach represents an alternative formulation of quantum mechanics. While classically the system follows only the classical path that minimizes the action, quantum mechanics implies that the system in fact takes every possible path. However, one important point that is not obvious is how the path integral over numbers (eigenvalues) can reproduce the commutation relations of operators. Moreover, we do not yet have a good understanding of the form of the quantum mechanical paths.

To address these questions, we consider so-called transition elements

$$\langle F\rangle = \int \mathcal{D}[q(t)]F[q(t)]\mathrm{e}^{\mathrm{i}S/\hbar}$$

where F is some functional of the path $q(t)$. Although we still have complex phases $\mathrm{e}^{\mathrm{i}S/\hbar}$ rather than probabilities, we may consider $\langle F\rangle$ to be an average of F along all possible paths between two points in space-time. In addition to the phase $\mathrm{e}^{\mathrm{i}S[q]/\hbar}$, each path is weighted by $F[q]$.

Following Feynman and Hibbs, we make the substitution $q(t) \mapsto q(t) + \eta(t)$, $\mathcal{D}[q(t) + \eta(t)] = \mathcal{D}[q(t)]$. Expanding to first order gives[15]

$$\begin{aligned}\langle F\rangle &= \int \mathcal{D}[q(t)]F[q(t)+\eta(t)]\mathrm{e}^{\mathrm{i}S[q(t)+\eta(t)]/\hbar} \\ &= \int \mathcal{D}[q(t)]F[q(t)]\mathrm{e}^{\mathrm{i}S[q(t)]/\hbar} + \int \mathcal{D}[q(t)]\left\{\int \mathrm{d}s\frac{\delta F}{\delta q(s)}\eta(s)\right\}\mathrm{e}^{\mathrm{i}S[q(t)]/\hbar} \\ &\qquad + \int \mathcal{D}[q(t)]F[q(t)]\left\{\int \mathrm{d}s\frac{\mathrm{i}}{\hbar}\frac{\delta S}{\delta q(s)}\eta(s)\right\}\mathrm{e}^{\mathrm{i}S[q(t)]/\hbar} + \ldots\end{aligned}$$

The first term on the rhs is just $\langle F\rangle$, so all the higher-order terms have to vanish. In particular, the first-order terms shown have to cancel for any $\eta(s)$, which gives the relation

$$\left\langle \frac{\delta F}{\delta q}\right\rangle = -\frac{\mathrm{i}}{\hbar}\left\langle F\frac{\delta S}{\delta q}\right\rangle . \tag{7}$$

[15] We use the following chain rule for the derivative of a function f of a functional F:

$$\frac{\delta f(F[g])}{\delta g(x)} = \left.\frac{\mathrm{d}f(z)}{\mathrm{d}z}\right|_{z=F[g]}\frac{\delta F[g]}{\delta g(x)}$$

where in our case $g(x) \to q(t)$, $f[F] \to \mathrm{e}^{\mathrm{i}S[q(t)]/\hbar}$, $F[f(x)] \to \int \mathrm{d}t L(q(t))$.

from which we can deduce several interesting results. To this end, we consider a particle in a potential, so that

$$S = \int \mathrm{d}t[\tfrac{1}{2}m\dot{q}^2 - V(q(t)]\,, \quad \frac{\delta S}{\delta q(t)} = -m\ddot{q} - V'(q)\,.$$

3.7.1 Newton's law

Setting $F = 1$, equation (7) implies

$$0 = -\frac{\mathrm{i}}{\hbar}\left\langle -m\ddot{q} - V'(q)\right\rangle$$

and hence

$$\langle m\ddot{q}\rangle = -\langle V'(q)\rangle\,.$$

3.7.2 Commutation relations

Next, we consider the discrete analogue of equation (7),

$$\left\langle \frac{\partial F}{\partial q_k}\right\rangle = -\frac{\mathrm{i}}{\hbar}\left\langle F\frac{\partial S}{\partial q_k}\right\rangle$$

and set $F = q_k$ to obtain

$$\begin{aligned}\langle 1\rangle &= -\frac{\mathrm{i}}{\hbar}\left\langle q_k \frac{\partial}{\partial q_k}\sum_j \Delta t\left[\frac{m}{2}\frac{(q_{j+1}-q_j)^2}{\Delta t^2} - V(q_j)\right]\right\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\left\langle q_k\left[m\frac{q_k - q_{k-1}}{\Delta t} + m\frac{q_k - q_{k+1}}{\Delta t} - \Delta t V'(q_k)\right]\right\rangle \\ &= \frac{\mathrm{i}}{\hbar}\left\langle m q_k\left[\frac{q_{k+1}-q_k}{\Delta t} - \frac{q_k - q_{k-1}}{\Delta t}\right] + \Delta t V'(q_k) q_k\right\rangle\end{aligned}$$

If the potential is sufficiently smooth, we can neglect the last term to find

$$\left\langle q_k \underbrace{m\frac{q_k - q_{k-1}}{\Delta t}}_{p(t=t_k-\Delta t/2)}\right\rangle - \left\langle \underbrace{m\frac{q_{k+1}-q_k}{\Delta t}}_{p(t=t_k+\Delta t/2)} q_k\right\rangle = \mathrm{i}\hbar\langle 1\rangle \tag{8}$$

which implies that $\langle pq\rangle \neq \langle qp\rangle$ (the result depends on the time-ordering of the operators), reminiscent of $[\hat{q},\hat{p}] = \mathrm{i}\hbar$.

3.7.3 Brownian motion

Since neighbouring time slices differ by Δt, we have to order Δt

$$\left\langle q_{k+1} m \frac{q_{k+1} - q_k}{\Delta t} \right\rangle \approx \left\langle q_k m \frac{q_k - q_{k-1}}{\Delta t} \right\rangle .$$

Replacing the rhs with the lhs in equation (8) gives

$$\left\langle m(q_{k+1} - q_k) \frac{q_{k+1} - q_k}{\Delta t} \right\rangle = \mathrm{i}\hbar \langle 1 \rangle$$

which we can rewrite as

$$\left\langle \left(\frac{q_{k+1} - q_k}{\Delta t} \right)^2 \right\rangle = \frac{\mathrm{i}\hbar}{m \Delta t} \langle 1 \rangle .$$

Because of the factor $1/\Delta t$ on the rhs, the average of the square of the velocity also has to scale as $1/\Delta t$, and hence diverge in the continuous limit $\Delta t \to 0$, $\langle v^2 \rangle \sim 1/\Delta\tau$. However, the velocity averaged over a short but finite time interval Δt is finite. At short distances, the paths are therefore continuous but not differentiable, and resemble those known from Brownian motion (self-similar, or fractal). This is not surprising in view of the discrete path integral, where q_k and $q_{k\pm1}$ are independent variables. In fact, the differentiable paths can be shown to be irrelevant (they have a Wiener measure of zero). The non-differentiable paths are essential for quantum effects, including the commutation relations. The path integral (especially in Euclidean time) therefore provides a connection between stochastic differential equations and random walks (known as the Feynman-Kac formula).

3.8 Relation to statistical mechanics

The path-integral approach reveals a remarkable relation between quantum mechanics and statistical mechanics. Let us recall that in statistical mechanics, the probability for the system to be in a state λ with energy E_λ is

$$p_\lambda = \frac{e^{-\beta E_\lambda}}{Z}$$

where $\beta = 1/(k_{\rm B}T)$ and Z is the partition function

$$Z = \sum_\lambda e^{-\beta E_\lambda} = \sum_\lambda \langle\lambda|\, {\rm e}^{-\beta\hat{H}}\, |\lambda\rangle = {\rm Tr}\, {\rm e}^{-\beta\hat{H}}\,.$$

Thinking of the coupled oscillator problem, we may be interested in the expectation value of the operator $\hat{n}_i$. The application of $\hat{n}_i$ to a state $|\lambda\rangle = |n_1^{(\lambda)}, n_2^{(\lambda)}, \ldots, n_N^{(\lambda)}\rangle$ gives the eigenvalue $n_i^{(\lambda)}$ (the number of excitations for lattice site/phonon mode i), and the thermal expectation value is given by

$$\langle\hat{n}_i\rangle = \sum_\lambda n_i^{(\lambda)} p_\lambda = \sum_\lambda \langle\lambda|\, \hat{n}_i\, |\lambda\rangle\, \frac{{\rm e}^{-\beta E_\lambda}}{Z} = \frac{1}{Z}\sum_\lambda \langle\lambda|\, \hat{n}_i {\rm e}^{-\beta\hat{H}}\, |\lambda\rangle = \frac{{\rm Tr}\, \hat{n}_i {\rm e}^{-\beta\hat{H}}}{{\rm Tr}\, {\rm e}^{-\beta\hat{H}}}\,.$$

An even more efficient way of calculating $\hat{n}_i$ relies on the quantity

$$Z(J) = {\rm Tr}\, {\rm e}^{-\beta\hat{H} + \sum_k J_k \hat{n}_k}\,,$$

the partition function of the Hamiltonian $\hat{H} + \beta^{-1}\sum_k J_k \hat{n}_k$ with sources J_k coupled to the oscillators. We have

$$\langle\hat{n}_i\rangle = \frac{1}{Z}\,\frac{\partial Z(J)}{\partial J_i}\bigg|_{J=0} = \frac{1}{Z(0)}\,\frac{\partial Z(J)}{\partial J_i}\bigg|_{J=0}\,.$$

From $Z(J)$, we can also obtain more complex expectation values such as the two-point correlation function

$$\langle\hat{n}_i\hat{n}_j\rangle = \frac{1}{Z(0)}\,\frac{\partial^2 Z(J)}{\partial J_i \partial J_j}\bigg|_{J=0}$$

or the m-point correlation function

$$\langle\hat{n}_{i_1}\hat{n}_{i_2}\ldots\hat{n}_{i_m}\rangle = \frac{1}{Z(0)}\,\frac{\partial^m Z(J)}{\partial J_{i_1}\ldots\partial J_{i_m}}\bigg|_{J=0}$$

For this reason, $Z(J)$ is called the generating function.

Returning to the example of a particle in a potential, the partition function in terms of position eigenstates takes the form

$$Z = \int \mathrm{d}q \, \langle q| \, \mathrm{e}^{-\beta \hat{H}} \, |q\rangle \ ,$$

the integrand of which has a strong resemblance to the amplitude ($t_a = 0$)

$$\langle q_b| \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} t_b \hat{H}} \, |q_a\rangle \ .$$

To have a complete match, we need to set $\mathrm{i}t_b = \beta\hbar$ and $q_a = q_b = q$. Since

$$\langle q_b| \, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} t_b \hat{H}} \, |q_a\rangle = \int \mathcal{D}[q(t)] \mathrm{e}^{\frac{\mathrm{i}}{\hbar} \int_0^{t_b} \mathrm{d}t L[q(t)]}$$

the amplitude $\langle q| \, \mathrm{e}^{-\beta \hat{H}} \, |q\rangle$ can be written as

$$\langle q| \, \mathrm{e}^{-\beta \hat{H}} \, |q\rangle = \int \mathcal{D}[q(t)] \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} \int_0^{-\mathrm{i}\beta\hbar} \mathrm{d}t L[q(t)]} \, .$$

where the time t varies in the range $[0, -\mathrm{i}\beta\hbar]$ on the imaginary axis. We now carry out the *Wick rotation* $t \mapsto \mathrm{i}t = \tau$ (corresponding to a rotation by $\pi/2$ in the complex plane) which leads to the following modifications:

- The time range in the exponent changes from $[0, -\mathrm{i}\beta\hbar]$ to $[0, \beta\hbar]$.
- We go from $\mathrm{d}t$ to $\mathrm{d}\tau = \mathrm{d}(\mathrm{i}t) = \mathrm{i}\mathrm{d}t$ by replacing $\mathrm{d}t$ with $-\mathrm{i}\mathrm{d}\tau$.
- The time derivative in the Lagrangian changes as well. Since

  $$\frac{\mathrm{d}}{\mathrm{d}\tau} = \frac{\mathrm{d}}{\mathrm{d}(\mathrm{i}t)} = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} \, , \quad \Rightarrow \frac{\mathrm{d}}{\mathrm{d}t} \mapsto \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\tau}$$

  the kinetic energy changes its sign,

  $$\frac{m}{2}\left(\frac{\mathrm{d}q}{\mathrm{d}t}\right)^2 \mapsto \frac{m}{2}\left(\mathrm{i}\frac{\mathrm{d}q}{\mathrm{d}\tau}\right)^2 = -\frac{m}{2}\left(\frac{\mathrm{d}q}{\mathrm{d}\tau}\right)^2 \, ,$$

  and we get the so-called Euclidean Lagrangian

  $$L_{\mathrm{E}} = \frac{m}{2}\left(\frac{\mathrm{d}q}{\mathrm{d}\tau}\right)^2 + V(q) \, .$$

With these changes, we can write the amplitude $\langle q|\, \mathrm{e}^{-\beta\hat{H}}\, |q\rangle$ as

$$\langle q|\, \mathrm{e}^{-\beta\hat{H}}\, |q\rangle = \int_{\substack{q(0)=q \\ q(\hbar\beta)=q}} \mathcal{D}[q(\tau)] \mathrm{e}^{-\frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau L_\mathrm{E}[q(\tau)]} \,.$$

The final step for the partition function is to include the integral/sum over the states $|q\rangle$, as implied by the trace. The structure of Z implies that we have a sum over all amplitudes $\langle q|\, \mathrm{e}^{-\beta\hat{H}}\, |q\rangle$, where $q(\tau)$ is a path that begins and ends at the same position q and extends over the imaginary time interval $[0, \beta\hbar]$. Instead of the boundary conditions $q(t_a) = q_a$ and $q(t_b) = q_b$ we hence have periodic boundary conditions (PBC) $q(\tau = 0) = q(\tau = \beta\hbar) = q$, with an integral over all possible q. The partition function then corresponds to[16]

$$Z = \int \mathrm{d}q\, \langle q|\, \mathrm{e}^{-\beta\hat{H}}\, |q\rangle = \int_\mathrm{PBC} \mathcal{D}[q(\tau)]\, \mathrm{e}^{-\frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau L_\mathrm{E}[q(\tau)]} \,.$$

Because $L_\mathrm{E} = T + V$, the integral $\int \mathrm{d}\tau L_\mathrm{E}$ can be regarded as the total energy of a 1D classical system of length $L = \beta\hbar$ and with Hamiltonian density $\mathcal{H} = \frac{m}{2}(\partial_\tau q)^2 + V(q)$. We can therefore write

$$Z = \int_\mathrm{PBC} \mathcal{D}[q]\, \mathrm{e}^{-\frac{1}{\hbar}\mathcal{E}[q]} \,.$$

with an energy functional $\mathcal{E}[q]$.

3.8.1 Comments

- We have found a mapping from a quantum system with D dimensions to a classical system in $D+1$ dimensions. For a single particle, we initially have a position variable $q \in \mathbb{R}$, corresponding to $D = 0$ (think in terms of a field $\phi = q$ at fixed location and time), which is then mapped to configurations $q(\tau)$ [or $\phi(\tau)$] defined on the 1D interval $[0, \beta\hbar]$. The additional dimension is imaginary time, and has a finite extent $[0, \beta\hbar]$ for finite temperatures. The paths are periodic with $q(\tau + \beta\hbar) = q(\tau)$ (for bosons).

[16] The additional integral over q gives N position integrals instead of $N-1$ in the discrete formulation of the path integral.

- The integrand has the form of a real Boltzmann weight, instead of the quantum mechanical phase factor $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S}$ found before. It decreases with increasing energy, thereby favouring low-energy paths/configurations. Strong fluctuations in the τ direction increase the energy because of the derivative $(\partial_\tau q)^2$. Similarly, if $V(q)$ is minimal at $q = 0$, configurations with $\langle q \rangle_\tau \neq 0$ have higher energy than those with $\langle q \rangle_\tau = 0$.

  To distinguish between thermal and quantum fluctuations, let us rewrite the exponent in terms of $\tau' = \tau/\hbar$:

  $$\frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau \left[\frac{m}{2}(\partial_\tau q)^2 + V(q)\right] = \int_0^{\beta} \mathrm{d}\tau' \left[\frac{1}{\hbar^2}\frac{m}{2}(\partial_{\tau'} q)^2 + V(q)\right]$$

  - If $m \to \infty$ or $\hbar \to 0$, fluctuations in the τ direction will be suppressed because of the large energy. The allowed configurations will hence be straight lines in τ, and fluctuations in imaginary time can be interpreted as quantum effects.
  - In the absence of any quantum fluctuations, the kinetic term drops out, and the functional integral becomes a regular integral:

    $$Z = \int \mathrm{d}q\, \mathrm{e}^{-\beta V(q)}\,,$$

    identical to the reduced classical partition function:

    $$Z_{\mathrm{cl}} = \int \mathrm{d}q \int \mathrm{d}p\, \mathrm{e}^{-\beta\left(\frac{p^2}{2m}+V(q)\right)} \sim \int \mathrm{d}q\, \mathrm{e}^{-\beta V(q)}.$$

- The Wick rotation corresponds to analytic continuation, and we can go back and forth between real and imaginary times (or even consider complex times). The Euclidean path integral is well defined mathematically (there are no oscillatory exponentials). For free particles, the integral measure is exactly the Wiener measure.

- Wick rotation turns the Schrödinger equation into a diffusion problem. The path integral provides a connection between diffusion and a random walk that has many applications, including financial markets. The relation between partial differential equations and random walks goes by the name of Feynman-Kac formula.

- In the imaginary-time representation, we can access the ground-state energy and the ground-state wave function from the propagator:

$$\langle q, \beta \mid q, 0 \rangle = \sum_n |\langle \phi_n \mid q \rangle|^2 \mathrm{e}^{-\beta E_n} \quad \stackrel{\beta\to\infty}{\longrightarrow} \quad |\phi_0(q)|^2 \mathrm{e}^{-\beta E_0}$$

  The ground state energy then follows from

$$E_0 = -\lim_{\beta\to\infty} \frac{1}{\beta} \ln Z = -\lim_{\beta\to\infty} \frac{1}{\beta} \ln \int_{\mathrm{PBC}} \mathcal{D}[q(\tau)]\, \mathrm{e}^{-\frac{1}{\hbar}\int_0^{\beta\hbar} \mathrm{d}\tau L_{\mathrm{E}}[q(\tau)]}$$

- We will later define a partition function and a generating functional for field theories, and express it in the form of a path (or functional) integral. This will allow us to calculate expectation values and correlation functions of quantum field theories at finite temperature (statistical field theory).

3.8.2 Partition function of the harmonic oscillator

To illustrate some of new concepts, let us calculate the partition function of the harmonic oscillator from the path integral. Setting $q_a = q_b = q$ and $t_b - t_a = -\mathrm{i}\hbar\beta$, we obtain from equation (6)

$$\langle q| \mathrm{e}^{-\beta\hat{H}} |q\rangle = \left(\frac{m\omega_0}{2\pi\hbar \sinh(\beta\hbar\omega_0)}\right)^{\frac{1}{2}} \exp\left[-\frac{1}{2}\frac{m\omega_0 q^2}{\hbar}\frac{2\cosh(\beta\hbar\omega_0)-2}{\sinh(\beta\hbar\omega_0)}\right] \quad (9)$$

To obtain the partition function, we integrate over q:[17]

$$\begin{aligned}
Z &= \int \mathrm{d}q\, \langle q| \mathrm{e}^{-\beta\hat{H}} |q\rangle \\
&= \left(\frac{m\omega_0}{2\pi\hbar \sinh(\beta\hbar\omega_0)}\right)^{\frac{1}{2}} \int \mathrm{d}q \mathrm{e}^{-\frac{1}{2}\frac{m\omega_0 q^2}{\hbar}\frac{2\cosh(\beta\hbar\omega_0)-2}{\sinh(\beta\hbar\omega_0)}} \\
&= \left(\frac{m\omega_0}{2\pi\hbar \sinh(\beta\hbar\omega_0)} \frac{2\pi\hbar \sinh(\beta\hbar\omega_0)}{m\omega_0[2\cosh(\beta\hbar\omega_0)-2]}\right)^{\frac{1}{2}} \\
&= \frac{1}{2\sinh(\beta\hbar\omega_0/2)} \\
&= \frac{\mathrm{e}^{-\beta\hbar\omega_0/2}}{1-\mathrm{e}^{-\beta\hbar\omega_0}} = \sum_{n=0}^{\infty} \mathrm{e}^{-\beta\hbar\omega_0(n+1/2)} = \sum_n \langle n| \mathrm{e}^{-\beta\hat{H}} |n\rangle \ .
\end{aligned}$$

[17] We use $\sin(\mathrm{i}x) = \mathrm{i}\sinh(x)$, $\cos(\mathrm{i}x) = \cosh(x)$, and $\cosh 2x - 1 = 2\sinh^2 x$.

3.9 Stationary phase approximation

In chapter 3.5, we were able to obtain the propagator of the quantum-mechanical free particle by considering a beam of paths near the classical path that contribute the same phase $\mathrm{e}^{\mathrm{i}S_c/\hbar}$. This approach can be generalized in the form of an expansion around the classical path in powers of $\hbar$ (rather than a weak-coupling expansion in a coupling strength). Because the action is stationary around the classical path, the expansion is around a saddle point. Since a stationary action implies a stationary phase, the method is referred to as either the saddle point approximation, the stationary phase approximation, or the semiclassical approximation.

To develop the method systematically, we consider a functional integral

$$\int \mathcal{D}[x(t)]\mathrm{e}^{-S[x]}\,, \quad \mathcal{D}[x(t)] = \lim_{N\to\infty}\prod_n \mathrm{d}x_n$$

which is the continuum limit of a path integral over variables $x_1, \ldots, x_N$. Let $\overline{x}(t)$ be the (only) path for which S is stationary,

$$\left.\frac{\delta S}{\delta x(t)}\right|_{x=\overline{x}} = 0\,.$$

We expand S in terms of the fluctuations around $\overline{x}$:[18]

$$S[x] = S[\overline{x}+y] = S[\overline{x}] + \frac{1}{2}\iint \mathrm{d}t\mathrm{d}t'\, y(t')\hat{A}(t,t')y(t) + \ldots$$

If the operator

$$\hat{A}(t,t') = \left.\frac{\delta^2 S[x]}{\delta x(t)\delta x(t')}\right|_{x=\overline{x}}$$

is positive definite, we can carry out the Gaussian integral to obtain

$$\int \mathcal{D}[x(t)]\mathrm{e}^{-S[x]} \sim \mathrm{e}^{-S[\overline{x}]}\,\det\left(\frac{\hat{A}}{2\pi}\right)^{-1/2}$$

[18] Compare this to the Taylor expansion for functions of many variables:

$$f(\vec{x}) = f(\vec{x}_0+\vec{y}) = f(\vec{x}_0) + \sum_j \left.\frac{\partial f(\vec{x})}{\partial x_j}\right|_{\vec{x}=\vec{x}_0} y_j + \frac{1}{2}\sum_j\sum_k \left.\frac{\partial^2 f(\vec{x})}{\partial x_j \partial x_k}\right|_{\vec{x}=\vec{x}_0} y_j y_k + \ldots$$

The second factor is known as the fluctuation determinant.

To apply this idea to the path integral for the propagator $\langle q_b| \, \mathrm{e}^{-\mathrm{i}\hat{H}t_b/\hbar} \, |q_a\rangle$ we write the paths as $q(t) = q_c(t) + r(t)$. Assuming that only even-order terms contribute (which is usually the case), we obtain the expansion

$$\frac{S}{\hbar} = \frac{S[q_c]}{\hbar} + \frac{1}{\hbar}\frac{1}{2}\int \mathrm{d}^2t \, r^2 S^{(2)} + \frac{1}{\hbar}\sum_{n=4}^{\infty}\frac{1}{n!}\int \mathrm{d}^n t \, r^n S^{(n)}$$

where $S^{(n)}$ denotes the n-th functional derivative of the action S. Because only q_c contributes in the classical limit $\hbar = 0$, we expect the fluctuation terms to vanish for $\hbar \to 0$. The fact that the expansion corresponds to a series expansion in the parameter $\hbar$ can be revealed in two ways:

1. A transformation of variables $r(t) \to \sqrt{\hbar}\widetilde{r}(t)$ eliminates the dependence on $\hbar$ in the quadratic term, and leaves the classical term unchanged (because it is independent of r):

   $$\frac{S}{\hbar} = \frac{S[q_c]}{\hbar} + \frac{1}{2}\int \mathrm{d}^2t \, \widetilde{r}^2 S^{(2)} + \frac{1}{\hbar}\sum_{n=4}^{\infty}\frac{1}{n!}\int \mathrm{d}^n t \, \hbar^{n/2}\widetilde{r}^n S^{(n)} \, .$$

   Since the action and its derivatives are classical objects and hence independent of $\hbar$, higher-order terms scale with $\mathcal{O}(\hbar^{n/2-1})$.

2. For the lowest (quadratic) order to be relevant, the phase difference relative to the classical action should be small, that is

   $$S^{(2)} r^2 \sim \hbar \quad \Longrightarrow r \sim \sqrt{\frac{\hbar}{S^{(2)}}}$$

   so that

   $$\frac{1}{\hbar}\int \mathrm{d}^n t \, r^n S^{(n)} \sim \frac{1}{\hbar}\int \mathrm{d}^n t \, \hbar^{n/2}\frac{S^{(n)}}{S^{(2)}} \sim \mathcal{O}(\hbar^{n/2-1}) \, .$$

For many applications, it is sufficient to include only the first correction, namely the term quadratic in the fluctuations $r(t)$:

$$\langle q_b| \, \mathrm{e}^{-\mathrm{i}\hat{H}t_b/\hbar} \, |q_a\rangle \simeq \mathrm{e}^{\mathrm{i}S[q_c]/\hbar}\mathcal{Z}^{(2)}$$

with the second-order (in the path fluctuations $r(t)$) correction[19]

$$\mathcal{Z}^{(2)} = \int_{\substack{r(0)=0\\ r(t_b)=0}} \mathcal{D}[r] \exp\left[\frac{\mathrm{i}}{2\hbar}\iint_0^{t_b} \mathrm{d}t\mathrm{d}t'\, r(t)\, \frac{\delta^2 S[q]}{\delta q(t)\delta q(t')}\bigg|_{q=q_c} r(t')\right].$$

Since the next ($n = 4$) term scales as $\mathcal{O}(\hbar^{4/2-1}) = \hbar$, we have

$$\langle q_b|\, \mathrm{e}^{-\mathrm{i}\hat{H}t_b/\hbar}\, |q_a\rangle = \mathrm{e}^{\mathrm{i}S[q_c]/\hbar}\mathcal{Z}^{(2)}(1+\mathcal{O}(\hbar))\,.$$

The second-order correction has the form of a Gaussian integral, which can be carried out. For a Lagrangian of the form $L = m\dot{q}^2/2 - V(q)$, we have

$$\iint_0^{t_b} \mathrm{d}t\mathrm{d}t'\, r(t)\, \frac{\delta^2 S[q]}{\delta q(t)\delta q(t')}\bigg|_{q=q_c} r(t') = -\int \mathrm{d}t\, r(t)[m\partial_t^2 + V''(q_c)]r(t)\,,$$

where $V'' = \partial_q^2 V(q)$ is the second derivative of the potential. Gaussian integration gives (up to normalization)

$$\mathcal{Z}^{(2)} = \frac{1}{\sqrt{\det(m\partial_t^2 + V''(q_c))}}$$

which involves the so-called *fluctuation operator*. The differential operator acts on the space of functions $r(t)$ with boundary conditions $r(0) = r(t_b) = 0$. Using the Van Vleck-Pauli-Morette formula, the propagator in the semi-classical approximation (and for a 1D problem) takes the form (see the book by Schulman)

$$\langle q_b|\, \mathrm{e}^{-\mathrm{i}\hat{H}t_b/\hbar}\, |q_a\rangle \approx \left(\frac{\mathrm{i}}{2\pi}\frac{\partial^2 S[q_c]}{\partial q_a \partial q_b}\right)^{1/2} \mathrm{e}^{\mathrm{i}S[q_c]/\hbar}\,.$$

For the harmonic oscillator we have $V''(q) = m\omega_0^2$ and the expansion in $\hbar$ terminates at the second order. Taking into account the fluctuation determinant hence gives the exact result for the propagator. For more general potentials $V(q)$, the second-order approximation corresponds to replacing the potential with a harmonic potential with the same curvature. Finally, if the action has several saddle points, the propagator contains a sum over the individual contributions.

[19] Because of the periodic boundary conditions, this factor looks like a partition function, hence the letter $\mathcal{Z}$.

3.10 Tunnelling and instantons

In this section, we use the path integral method developed above to understand the problem of a particle (or, equivalently a zero-dimensional scalar field) in a double-well potential $V(q)$. We have encountered such a potential before in the context of spontaneous symmetry breaking. It turns out that this rather simple problem plays a role in many areas of theoretical physics.

Consider a particle with Lagrangian

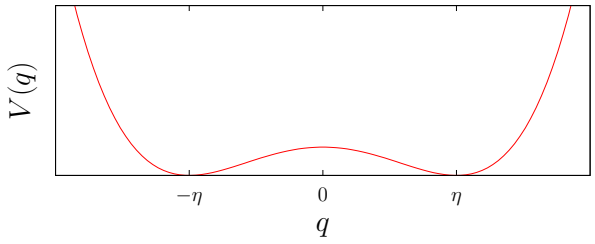
$$L = \tfrac{1}{2} m\dot{q}^2 - V(q)$$

with a potential of the form

$$V(q) = \lambda(q-\eta)^2(q+\eta)^2 = \lambda(q^2-\eta^2)^2$$

so that

$$V(\pm\eta) = 0\,, \quad V'(\pm\eta) = 0\,, \quad V''(\pm\eta) = 8\lambda\eta^2 \equiv m\omega^2\,.$$



The reason for setting $8\lambda\eta^2 \equiv m\omega^2$ is that for $q \approx \pm\eta$ we can approximate the problem with a harmonic potential of the same curvature, $V_{\rm h}^{\pm} = m\omega_0^2(q\pm\eta)^2$.

Classically, a particle which is at $q = -\eta$ at time $t_i = -t_0/2$ and has an energy smaller than the barrier between the two minima will stay near $q = -\eta$ forever. Quantum effects ($\Delta E \sim \hbar/\Delta t$) give rise to a finite amplitude for the particle to tunnel through the barrier. In particular, in the absence of symmetry breaking, the quantum mechanical ground state is a symmetric superposition with equal probability for the particle to be near $-\eta$ and $+\eta$.

Our goal is to calculate the amplitudes for the particle to either stay where it is or to tunnel using the path integral within the semiclassical (stationary phase) approximation. The amplitudes of interest are

$$G(q_b, t_0/2, q_a, -t_0/2) = \langle q_b | \, \mathrm{e}^{-\mathrm{i}\hat{H}t_0/\hbar} \, | q_a \rangle$$

where $q_a, q_b = \pm\eta$ and we will eventually consider the limit $t_0 \to \infty$.

The semiclassical approximation is based on the idea of the amplitude being dominated by the classical path, while quantum effects are taken into account in terms of the fluctuation determinant. However, for the double-well potential, there are no classical solutions that connect the two minima. To proceed, we therefore make use of the Wick rotation $t \mapsto -\mathrm{i}\tau$, The amplitude

$$G_E(q_b, \tau_0/2, q_a, -\tau_0/2) = \langle q_b | \, \mathrm{e}^{-\tau_0\hat{H}} \, | q_a \rangle$$

can be expressed as a Euclidean path integral

$$G_E(q_b, \tau_0/2, q_a, -\tau_0/2) = \int_{\substack{q(-\tau_0/2)=q_a \\ q(+\tau_0/2)=q_b}} \mathcal{D}[q(\tau)] \exp\left[-\frac{1}{\hbar} \int_{-\tau_0/2}^{\tau_0/2} L_E \right]$$

with the Euclidean Lagrangian

$$L_E = \tfrac{1}{2} m \dot{q}^2 + V(q) \, .$$

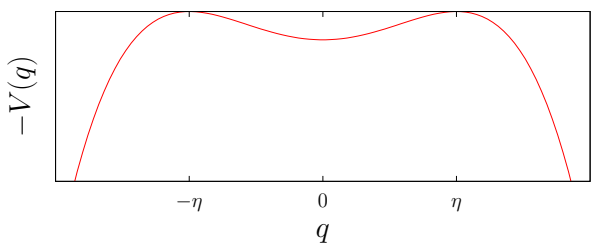
In Euclidean time, the stationary phase approximation corresponds to

$$G_E(\pm\eta, \tau_0/2, -\eta, -\tau_0/2) = N \mathrm{e}^{-S[q_c]/\hbar} \left[\det\left(-\partial_\tau^2 + V''(q_c) \right) \right]^{-1/2}$$

To calculate the quantity $\mathrm{e}^{-S[q_c]/\hbar}$ we have to find the (classical) solutions to

$$m\ddot{q} = V'(q) \equiv -V_E'(q) \, .$$

As a result of the Wick rotation, we have ended up with a problem in the inverted potential $V_E = -V$. It has maxima at $q = \pm\eta$, so that we can easily find classical solutions connecting these two points. Once we have the solutions, we can revert to time t using analytic continuation.



We first consider the case of $q_a = q_b$. The corresponding amplitude from the stationary phase approximation is

$$\langle \pm\eta |\, \mathrm{e}^{-\tau_0 \hat{H}}\, | \pm\eta \rangle = N \mathrm{e}^{-S[q_c]/\hbar} \left[\det\left(-\partial_\tau^2 + m\omega^2 \right) \right]^{-1/2}$$

where we used $V''(\pm\eta) = m\omega^2$. This expression corresponds to the exact propagator for a harmonic potential $V(q) = m\omega^2(q \pm \eta)^2$, and has previously been calculated. Setting $\omega_0 = \omega$, $q = q_b - q_a = 0$, $\beta = \tau_0$ in equation (9) gives

$$\langle \pm\eta |\, \mathrm{e}^{-\tau_0 \hat{H}}\, | \pm\eta \rangle = \left(\frac{m\omega}{2\pi\hbar \sinh(\hbar\tau_0\omega)} \right)^{\frac{1}{2}} = \left(\frac{m\omega}{\hbar\pi} \right)^{\frac{1}{2}} \frac{1}{\sqrt{2\sinh(\hbar\tau_0\omega)}}$$

The path integral formulation allows us to use our knowledge of classical mechanics: in Euclidean time, we have an inverted potential with a maximum at $q = 0$. The physics is dominated by the classical path(s) that minimize(s) the action. If we are interested in the amplitude $\langle q_0, \tau_0/2 \,|\, q_0, -\tau_0/2 \rangle$, the only possible classical path with a finite action in the limit $\tau_0 \to \infty$ is that for which the particle remains at $q_0 = 0$ for all τ. For $q_0 \neq 0$, the particle will roll off to infinity and never return, leading to an infinite action for $\tau_0 \to \infty$. Regardless of the exact form of V, we know that $S[q_c] = 0$ because $q_c(\tau) = q_0 = 0$. For the double-well potential, we have $q_c(\tau) = \pm\eta$.

Let us consider the limit $\tau_0 \to \infty$ (for which the ground state will dominate) by using the expansion $(1-x)^{-1/2} \approx 1 + x/2$ to get

$$\frac{1}{\sqrt{2\sinh(\hbar\tau_0\omega)}} = \frac{\mathrm{e}^{-\hbar\tau_0\omega/2}}{\sqrt{1 - \mathrm{e}^{-2\hbar\tau_0\omega}}} = \mathrm{e}^{-\hbar\tau_0\omega/2}(1 + \tfrac{1}{2}\mathrm{e}^{-2\hbar\tau_0\omega} + \dots)$$

The amplitude then takes the form

$$\langle \pm\eta |\, \mathrm{e}^{-\tau_0 \hat{H}}\, | \pm\eta \rangle = \left(\frac{m\omega}{\hbar\pi} \right)^{\frac{1}{2}} \mathrm{e}^{-\hbar\tau_0\omega/2}(1 + \tfrac{1}{2}\mathrm{e}^{-2\hbar\tau_0\omega} + \dots)$$

from which we identify the ground-state energy $E_0 = \hbar\omega/2$ and the first contribution from excited states. The prefactor corresponds to $|\psi_0(0)|^2$ with the real-space wave function of the harmonic oscillator

$$\psi_n(q) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\hbar\pi} \right)^{\frac{1}{4}} \mathrm{e}^{-\frac{m\omega^2 q^2}{2\hbar}} H_n(\sqrt{\tfrac{m\omega}{\hbar}} q)\,,$$

where H_n is the n-th Hermite polynomial and $H_0 = 1$. For large times τ_0, we can hence approximate the amplitude as

$$\langle \pm\eta | \, \mathrm{e}^{-\tau_0 \hat{H}} \, | \pm\eta \rangle \approx \left(\frac{m\omega}{\hbar\pi} \right)^{\frac{1}{2}} \mathrm{e}^{-\hbar\tau_0\omega/2}$$

Apart from the stationary solutions where the particle stays at its initial position, we are also interested in the amplitude for tunnelling between the minima, described by the amplitude $G_E(+\eta, \tau_0/2, -\eta, -\tau_0/2) = \langle \eta | \, \mathrm{e}^{-\tau_0 \hat{H}} \, | -\eta \rangle$. We will again consider the limit $\tau_0 \to \infty$, so that classically we consider a particle starting at $q = -\eta$ at $\tau = -\infty$ and ending at $q = +\eta$ for $\tau = +\infty$. To derive a classical solution for this process, we use energy conservation:

$$E = \tfrac{1}{2} m \dot{q}^2 - V(q) = const.$$

Since our potential has the property $V(\pm\eta) = 0$, $E = 0$. Therefore, we have

$$\frac{\mathrm{d}q}{\mathrm{d}\tau} = \sqrt{\frac{2V}{m}} = \pm\sqrt{\frac{2\lambda}{m}}(q^2 - \eta^2)$$

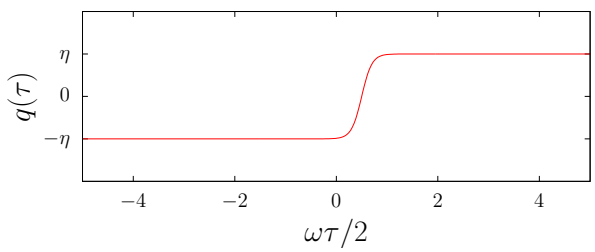
which can be integrated and gives (using $\sqrt{2\lambda/m} = \omega/2\eta$)

$$q(\tau) = \eta \tanh\left(\mp \tfrac{1}{2}\omega\tau + C \right) .$$

The sign can be fixed to + using the boundary condition $q(\tau \to \infty) = +\eta$, and the constant C determines the point in time when the particle tunnels. We rewrite the solution as

$$q_{\mathrm{inst}}(\tau) = \eta \tanh\left[\frac{\omega(\tau - \tau_c)}{2} \right] .$$

The derivative is $\dot{q}/\eta = \{2\Delta \cosh^2[(\tau - \tau_c)/(2\Delta)]\}^{-1}$ which becomes $\delta(\tau - \tau_c)$ in the limit $\Delta = \omega^{-1} \to 0$. The tunnelling takes place on a time scale Δ and for $\tau_0 \gg \Delta$ may be considered as instantaneous. Because it describes a transition well localized in time, q_{inst} is known as an instanton solution (instantons are essentially domain walls in the time domain).



Having found a classical solution that connects $-\eta$ and η, we consider the amplitude. Except for the short interval around τ_c, the particle is in one of the minima. Hence, we can assume that the propagator is essentially that for a particle that stays at $\eta = \pm 1$, with a correction K due to the tunnelling:

$$\langle \pm\eta | \, \mathrm{e}^{-\tau_0 \hat{H}} \, | \mp\eta \rangle \approx \left(\frac{m\omega}{\hbar\pi} \right)^{\frac{1}{2}} \mathrm{e}^{-\hbar\tau_0\omega/2} \, \mathrm{e}^{-S[q_{\mathrm{inst}}]/\hbar} \, K \, . \tag{10}$$

While we shall not do the explicit calculation,[20] we know from the stationary phase approximation that

$$\langle \pm\eta | \, \mathrm{e}^{-\tau_0 \hat{H}} \, | \mp\eta \rangle \approx N \, \mathrm{e}^{-S[q_{\mathrm{inst}}]/\hbar} \, \left[\det \left(-\partial_\tau^2 + V''(q_{\mathrm{inst}}) \right) \right]^{-1/2}$$

so that K corresponds to the ratio

$$K = \left[\frac{\det \left(-\partial_\tau^2 + V''(q_{\mathrm{inst}}) \right)}{\det \left(-\partial_\tau^2 + m\omega^2 \right)} \right]^{-1/2} \, .$$

The action $S[q_{\mathrm{inst}}] \equiv S_0$ can be calculated for a given q_{int} but the following considerations are independent of the exact form of the instanton. For completeness:

$$S[x_{\mathrm{inst}}] = \int_{-\infty}^{\infty} \mathrm{d}\tau \, \left[\tfrac{1}{2} m \dot{x}^2 + V(x) \right] = \int_{-\infty}^{\infty} \mathrm{d}\tau \, m \dot{x}^2$$

which can be written as

$$S[x_{\mathrm{inst}}] = m \int_{-\infty}^{\infty} \mathrm{d}\tau \frac{\mathrm{d}x}{\mathrm{d}\tau} \frac{\mathrm{d}x}{\mathrm{d}\tau} = m \int_{-\eta}^{\eta} \mathrm{d}x \, \dot{x}(x) = -m \int_{-\eta}^{\eta} \mathrm{d}x \, \sqrt{\frac{2V}{m}}$$

and can be evaluated to give

$$S[x_{\mathrm{inst}}] = \frac{\omega^3 m^2}{12\lambda} \, .$$

Just like a ferromagnet can have many domains separated by domain walls, a particle can tunnel between $-\eta$ and η more than once. Assuming that the time between tunnelling events is much larger than Δ, we can approximate these events as independent random events (instanton gas). As before, except

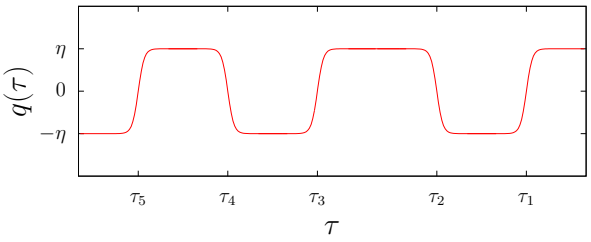
[20] See the books of Zinn-Justin or Altland and Simons for more details.

for the short periods of tunnelling, the particle sits in one of the potential minima. The amplitude for the case of n instantons will hence have the form

$$\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}} \mathrm{e}^{-\hbar\tau_0\omega/2}\, \mathrm{e}^{-nS_0/\hbar}\, K^n\,.$$

The times τ_n where tunnelling takes place (corresponding to the centres of the instanton solutions) are random variables to be integrated over. Let us number the tunnelling times from right (later times) to left (earlier times):

$$-\frac{\tau_0}{2} \le \tau_n \le \tau_{n-1} \le \cdots \le \tau_1 \le \frac{\tau_0}{2}$$



The first event can occur anywhere in the interval $[-\tau_0/2, \tau_0/2]$. The second event is then restricted to $[-\tau_0/2, \tau_1]$, and so on. We hence have

$$\int_{-\tau_0/2}^{\tau_0/2} \mathrm{d}\tau_1 \int_{-\tau_0/2}^{\tau_1} \mathrm{d}\tau_2 \int_{-\tau_0/2}^{\tau_2} \mathrm{d}\tau_3 \cdots \int_{-\tau_0/2}^{\tau_{n-1}} \mathrm{d}\tau_n$$

which is identical to

$$\frac{1}{n!} \int_{-\tau_0/2}^{\tau_0/2} \mathrm{d}\tau_1 \int_{-\tau_0/2}^{\tau_0/2} \mathrm{d}\tau_2 \int_{-\tau_0/2}^{\tau_0/2} \mathrm{d}\tau_3 \cdots \int_{-\tau_0/2}^{\tau_0/2} \mathrm{d}\tau_n = \frac{\tau_0^n}{n!}$$

The total amplitude is the sum over all possible values of n (instanton numbers), with the restriction that we need n even for, for example, $\langle -\eta|\, \mathrm{e}^{-\tau_0\hat{H}}\, |-\eta\rangle$ and n odd for $\langle +\eta|\, \mathrm{e}^{-\tau_0\hat{H}}\, |-\eta\rangle$:

$$\langle -\eta|\, \mathrm{e}^{-\tau_0\hat{H}}\, |-\eta\rangle = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}} \mathrm{e}^{-\hbar\tau_0\omega/2} \sum_{n=0,2,\ldots} \frac{\left(K\tau_0 \mathrm{e}^{-S_0/\hbar}\right)^n}{n!}$$

$$\langle +\eta|\, \mathrm{e}^{-\tau_0\hat{H}}\, |-\eta\rangle = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}} \mathrm{e}^{-\hbar\tau_0\omega/2} \sum_{n=1,3,\ldots} \frac{\left(K\tau_0 \mathrm{e}^{-S_0/\hbar}\right)^n}{n!}$$

Using

$$\cosh x = \sum_{n=0}^{\infty} \frac{x^{2n}}{(2n)!}\,, \quad \sinh x = \sum_{n=0}^{\infty} \frac{x^{2n+1}}{(2n+1)!}$$

we obtain

$$\langle \pm\eta |\, \mathrm{e}^{-\tau_0 \hat{H}}\, |-\eta\rangle = \frac{1}{2}\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}} \mathrm{e}^{-\hbar\tau_0\omega/2}\left[\mathrm{e}^{K\tau_0 \mathrm{e}^{-S_0/\hbar}} \mp \mathrm{e}^{-K\tau_0 \mathrm{e}^{-S_0/\hbar}}\right].$$

We can infer that for large τ_0 the amplitude is dominated by two low-energy contributions (one in which we end up at $-\eta$, the other in which we end up at $+\eta$ for $\tau \to \infty$) with energies

$$E_\pm = \tfrac{1}{2}\hbar\omega \pm \hbar K \mathrm{e}^{-S_0/\hbar}\,.$$

The first term is the energy for a particle that just sits in one of the minima. The second term is related to the tunnelling between the minima. The two states with energies $E_\pm$ correspond to the symmetric and antisymmetric combination of the oscillator ground states. Note that instantons cannot be obtained from a small perturbation around the configurations without tunnelling. A configuration with n instantons cannot be smoothly deformed into one with $n \pm 1$. States with different winding numbers n are hence topologically distinct.

Let us reconcile this finding with quantum mechanics. We denote the states with the particle localized in one of the minima as $|\pm\eta\rangle$ and the corresponding energy as $\langle\eta|\,\hat{H}\,|\eta\rangle = \langle -\eta|\,\hat{H}\,|-\eta\rangle = U$. The tunnelling between the minima is related to matrix elements $\langle -\eta|\,\hat{H}\,|\eta\rangle = \langle\eta|\,\hat{H}\,|-\eta\rangle = -V$. The problem is hence equivalent two a two-level system with Hamiltonian matrix

$$H = \begin{pmatrix} U & -V \\ -V & U \end{pmatrix}$$

with eigenstates

$$|+\rangle = \frac{1}{\sqrt{2}}\left(|\eta\rangle + |-\eta\rangle\right), \quad E_+ = U - V\,,$$
$$|-\rangle = \frac{1}{\sqrt{2}}\left(|\eta\rangle - |-\eta\rangle\right), \quad E_- = U + V\,.$$

With the path integral, we have managed to describe quantum tunnelling between classical minima (vacuum states) using a picture of classical paths in imaginary time.

4 Path integral for fields and many particles

In this section, we extend the path integral to the case of field theories and many-particle systems. For the latter, we may consider a general Hamiltonian for N particles:

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} v(\hat{q}_i - \hat{q}_j)$$

The Feynman path integral may be formulated with the help of N-particle basis states $|q_1, q_2, \ldots, q_N\rangle$ to obtain the partition function

$$Z = \frac{1}{N!} \int \prod_{i=1}^{N} \mathrm{d}q_i \, \langle q_1, q_2, \ldots, q_N | \, \mathrm{e}^{-\beta \hat{H}} \, | q_1, q_2, \ldots, q_N \rangle$$

as a functional integral over all possible configurations

$$Z = \frac{1}{N!} \sum_P \zeta^P \int_{\substack{q_1(\beta) = q_{P(1)}(0) \\ \vdots \\ q_N(\beta) = q_{P(N)}(0)}} \mathcal{D}[q_1(\tau) \ldots q_N(\tau)] \times \mathrm{e}^{-\int_0^\beta \mathrm{d}\tau \left[\sum_{i=1}^N \frac{m}{2} \dot{q}(\tau)^2 + \frac{1}{2} \sum_{i \neq j} v(q_i(\tau) - q_j(\tau)) \right]} .$$

Here P is the permutation operator mapping the indices $1, 2, \ldots, N$ to $P(1), P(2), \ldots, P(N)$, and $\zeta = \pm 1$ for bosons (fermions).

While this representation can in principle be used for calculations or numerical simulations, a representation of $\hat{H}$ in terms of creation/annihilation operators turns out to be much more useful. The path integral can then be formulated using coherent states (bosons) or Grassmann variables (fermions), leading to a functional integral over field configurations.

4.1 Second quantization

To express a general many-particle Hamiltonian in terms of creation and annihilation operator, we have to slightly expand upon the discussion in chapter 1. The basic idea remains the same: instead of specifying which particle is in which state (impossible if we have identical particles), we want

to use a basis of states that specify how many particles/excitations are in each allowed state. For the coupled harmonic oscillators, we arrived at

$$|n_1, n_2, \ldots, n_N\rangle = \frac{1}{\sqrt{n_1! n_2! \cdots n_N!}} (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \cdots (a_N^\dagger)^{n_N} \underbrace{|0, 0, \ldots, 0\rangle}_{|0\rangle}$$

where the operator $a_i^\dagger$ creates a particle/excitation in level i, and $\hat{n}_i = a_i^\dagger a_i$ counts the number of particles/excitations in level i. While we obtained a description in terms of excitations of the allowed states for the harmonic oscillator, creation and annihilation operators may correspond to actual particles (electrons, bosonic atoms, ...).

A fundamental concept for many-particle quantum systems is the fact that identical particles cannot be distinguished, and that the exchange of identical particles cannot have any effect on observables. For example, the wave function for two particles can only change by a phase upon interchanging the particles,

$$\psi(x_2, x_1) = \lambda \psi(x_1, x_2) = \mathrm{e}^{\mathrm{i}\theta} \psi(x_1, x_2)\,,$$

in order to preserve the probability density $|\psi|^2$ and expectation values. The spin-statistics theorem tells us that for particles with integer spin (bosons) $\lambda = 1$ so that

$$\psi(x_2, x_1) = \psi(x_1, x_2)\,.$$

For particles with half-integer spin (fermions), we have $\lambda = -1$ and

$$\psi(x_2, x_1) = -\psi(x_1, x_2)\,.$$

Because the particles are identical, the many-particle wave function has to be independent of the way we label the particles. This is achieved by summing over all possible ways of putting N particles into N single-particle states.

For bosons (where more than one particle can occupy a given state/level), we define a symmetrized many-particle wave function as

$$\psi^{(+)}_{n_1 n_2 \ldots n_N}(x_1, x_2, \ldots, x_N) \equiv \sqrt{\frac{1}{N! \prod_j n_j!}} \sum_P \psi_{P1}(x_1) \psi_{P2}(x_2) \cdots \psi_{PN}(x_N)\,.$$

Here, P denotes permutation of the indices $i = 1, \ldots, N$. This wave function is symmetric under the exchange of particles. Hence, even though we have

numbered the particles for bookkeeping, the numbering must not have any physical consequences. This is achieved by symmetrization.[21]

For fermions, an antisymmetric wave function for N particles (with $n_i = 0, 1$) is given by

$$\psi^{(-)}_{n_1 n_2 \ldots n_N}(x_1, x_2, \ldots, x_N) \equiv \frac{1}{\sqrt{N!}} \sum_P (-1)^P \psi_{P1}(x_1) \psi_{P2}(x_2) \cdots \psi_{P(N)}(x_N) \,,$$

which can be written as a Slater determinant of single-particle states:

$$\psi^{(-)}_{n_1 n_2 \ldots n_N}(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_1}(x_2) & \cdots & \psi_{n_1}(x_N) \\ \psi_{n_2}(x_1) & \psi_{n_2}(x_2) & \cdots & \psi_{n_2}(x_N) \\ \vdots & \vdots & \vdots & \vdots \\ \psi_{n_N}(x_1) & \psi_{n_N}(x_2) & \cdots & \psi_{n_N}(x_N) \end{vmatrix} .$$

The use of creation/annihilation operators allows to account for the particle statistics in terms of commutation relations. Consider a state of two particles with momenta p_1 and p_2, which can be created in two ways:

$$a^\dagger_{p_1} a^\dagger_{p_2} |0\rangle = a^\dagger_{p_1} |01\rangle \sim |11\rangle \;, \quad a^\dagger_{p_2} a^\dagger_{p_1} |0\rangle = a^\dagger_{p_2} |10\rangle \sim |11\rangle$$

Because the particles are identical, the final state has to be the same up to a sign $\lambda = \pm 1$. For bosons we have $\lambda = 1$, which implies that

$$a^\dagger_{p_1} a^\dagger_{p_2} = a^\dagger_{p_2} a^\dagger_{p_1} \quad \leftrightarrow \quad a^\dagger_{p_1} a^\dagger_{p_2} - a^\dagger_{p_2} a^\dagger_{p_1} = 0 \quad \leftrightarrow \quad [a^\dagger_{p_1}, a^\dagger_{p_2}] = 0$$

Moreover, we have (cf. the harmonic oscillator)

$$[a_{p_1}, a_{p_2}] = 0 \,, \quad [a_{p_1}, a^\dagger_{p_2}] = \delta_{p_1, p_2} \,.$$

The operators act on the so-called Fock space, a tensor product of Hilbert spaces $\mathcal{F}_n$ with particle numbers n, $\mathcal{F} = \bigotimes_{n=0}^\infty \mathcal{F}_n$:

$$a^\dagger_i |n_1 \ldots n_i \ldots\rangle = \sqrt{n_i + 1} \, |n_1 \ldots n_i + 1 \ldots\rangle$$
$$a_i |n_1 \ldots n_i \ldots\rangle = \sqrt{n_i} \, |n_1 \ldots n_i - 1 \ldots\rangle$$

[21] Returning to the many-particle state for our system of coupled oscillators, we have

$$|n_1, n_2, \ldots, n_N\rangle = \frac{1}{\sqrt{N! \prod_i n_i!}} \sum_P |n_{P1}\rangle \otimes |n_{P2}\rangle \otimes |n_{PN}\rangle \;.$$

A general basis state in Fock space is given by

$$|n_1, n_2, \ldots\rangle = \prod_m \frac{1}{\sqrt{n_m!}} (a_m^\dagger)^{n_m} |0\rangle \ .$$

The commutation relations imply that for bosons the order in which we populate the levels is irrelevant:

$$a_{p_1}^\dagger a_{p_2}^\dagger |0\rangle = a_{p_2}^\dagger a_{p_1}^\dagger |0\rangle = |11\rangle$$

In the case of fermions we have $\lambda = -1$ which gives the commutation relations

$$\{c_i^\dagger, c_j^\dagger\} = 0 \,, \quad \{c_i, c_j\} = 0 \,, \quad \{c_i, c_j^\dagger\} = \delta_{ij}$$

with the anticommutator $\{A, B\} = AB + BA$. Note that for the same state $i = j$ we have

$$\{c_i^\dagger, c_i^\dagger\} = c_i^\dagger c_i^\dagger + c_i^\dagger c_i^\dagger = 0 \quad \rightarrow \quad c_i^\dagger c_i^\dagger = 0 \,,$$

the operator version of the Pauli principle! Because fermion operators anti-commute, the order in which we add particles to the vacuum does matter:

$$c_1^\dagger c_2^\dagger |0\rangle = |11\rangle \ , \quad c_2^\dagger c_1^\dagger |0\rangle = -|11\rangle$$

To properly account for the statistics of fermionic particles, we have to choose a convention for the order in which we let the operators act on states and stick to it. A popular choice is

$$\begin{aligned} c_i^\dagger |n_1 \ldots n_i \ldots\rangle &= (-1)^{\sum_i} \sqrt{1 - n_i} \, |n_1 \ldots n_i + 1 \ldots\rangle \\ c_i \, |n_1 \ldots n_i \ldots\rangle &= (-1)^{\sum_i} \sqrt{n_i} \, |n_1 \ldots n_i - 1 \ldots\rangle \end{aligned}$$

with the Fermi sign $(-1)^{\Sigma_i} = (-1)^{n_1 + n_2 + \cdots + n_{i-1}}$.

In the continuum limit, the commutation relations become ($\vec{p}$ is the 3-momentum)

$$[a_{\vec{p}}^\dagger, a_{\vec{q}}^\dagger] = 0 \,, \quad [a_{\vec{p}}, a_{\vec{q}}] = 0 \,, \quad [a_{\vec{p}}, a_{\vec{q}}^\dagger] = \delta^{(3)}(\vec{p} - \vec{q})$$

$$\{c_{\vec{p}}^\dagger, c_{\vec{q}}^\dagger\} = 0 \,, \quad \{c_{\vec{p}}, c_{\vec{q}}\} = 0 \,, \quad \{c_{\vec{p}}, c_{\vec{q}}^\dagger\} = \delta^{(3)}(\vec{p} - \vec{q})$$

The previously encountered field operators, which create/destroy particles at a specific point in space, are given by[22]

$$\hat{\psi}^\dagger(\vec{x}) = \frac{1}{\sqrt{V}} \sum_{\vec{p}} a^\dagger_{\vec{p}} \mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{x}}\,, \quad \hat{\psi}(\vec{x}) = \frac{1}{\sqrt{V}} \sum_{\vec{p}} a_{\vec{p}}\, \mathrm{e}^{\mathrm{i}\vec{p}\cdot\vec{x}}$$

and have the expected commutation relations for bosons

$$[\hat{\psi}(\vec{x}), \hat{\psi}(\vec{y})] = [\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{y})] = 0\,, \quad [\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{y})] = \delta^{(3)}(\vec{x}-\vec{y})$$

and fermions

$$\{\hat{\psi}(\vec{x}), \hat{\psi}(\vec{y})\} = \{\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{y})\} = 0\,, \quad \{\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{y})\} = \delta^{(3)}(\vec{x}-\vec{y})\,.$$

Now that we know how to write properly symmetrized many-particle states in second quantization, we need to consider operators. We begin with a single-particle operator such as the kinetic energy. With the help of complete sets of (single-particle) states $\{|\psi_n\rangle\}$, we obtain

$$\hat{A} = \sum_{n,m} |\psi_n\rangle \langle\psi_n| \hat{A} |\psi_m\rangle \langle\psi_m| = \sum_{n,m} \langle\psi_n| \hat{A} |\psi_m\rangle |\psi_n\rangle \langle\psi_m| = \sum_{n,m} A_{nm} |\psi_n\rangle \langle\psi_m|$$

where we defined the matrix element $A_{nm} = \langle\psi_n| \hat{A} |\psi_m\rangle$. The generalization to the Fock space of many-particle states turns out to be given by

$$\hat{A} = \sum_{n,m} A_{nm} a^\dagger_n a_m$$

where A_{nm} is the same matrix element as above, and $a^\dagger_n$ creates a particle in the state $|\psi_n\rangle$. The operator A is hence described in terms of single-particle scattering processes with matrix elements A_{nm}. Here, the indices n, m also include the spin directions. For example, the kinetic energy operator $\hat{T} = \sum_j \frac{\hat{p}_j^2}{2m}$ (the sum is over all particles) in momentum representation reads

$$\hat{T} = \sum_{\vec{p}_1,\vec{p}_2,\sigma_1,\sigma_2} \left\langle \vec{p}_1, \sigma_1 \left| \frac{\hat{p}^2}{2m} \right| \vec{p}_2, \sigma_2 \right\rangle a^\dagger_{\vec{p}_1,\sigma_1} a_{\vec{p}_2,\sigma_2} = \sum_{\vec{p},\sigma} \frac{p^2}{2m} a^\dagger_{\vec{p},\sigma} a_{\vec{p},\sigma} = \sum_{\vec{p},\sigma} \epsilon_{\vec{p},\sigma} \hat{n}_{\vec{p},\sigma}\,.$$

[22] Here we consider a finite volume V so that the momenta are discrete.

We can also write the kinetic energy in real space using the field operators,

$$\hat{T} = -\frac{1}{2m} \sum_{\sigma} \int \mathrm{d}\vec{x}\, \hat{\psi}^{\dagger}_{\sigma}(\vec{x}) \nabla^2_{\vec{x}} \hat{\psi}_{\sigma}(\vec{x})\,,$$

which follows from partial integration and the expansions

$$a^{\dagger}_{\vec{p},\sigma} = \frac{1}{\sqrt{V}} \int \mathrm{d}\vec{x}\, \mathrm{e}^{\mathrm{i}\vec{p}\cdot\vec{x}} \hat{\psi}^{\dagger}_{\sigma}(\vec{x})\,, \quad a_{\vec{p},\sigma} = \frac{1}{\sqrt{V}} \int \mathrm{d}\vec{x}\, \mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{x}} \hat{\psi}_{\sigma}(\vec{x})\,.$$

Similarly, a general two-particle operator takes the form

$$\hat{A} = \sum_{klnm} A_{klnm} a^{\dagger}_k a^{\dagger}_l a_m a_n\,.$$

For the case of a two-particle interaction potential $\hat{V} = \frac{1}{2}\sum_{i\neq j} v(\hat{\vec{r}}_i - \hat{\vec{r}}_j)$, we can write in terms of field operators

$$\hat{V} = \frac{1}{2} \sum_{\sigma_1,\sigma_2} \iint \mathrm{d}\vec{x}\mathrm{d}\vec{y}\, \hat{\psi}^{\dagger}_{\sigma_1}(\vec{x}) \hat{\psi}^{\dagger}_{\sigma_2}(\vec{y}) v(\vec{x}-\vec{y}) \hat{\psi}_{\sigma_2}(\vec{y}) \hat{\psi}_{\sigma_1}(\vec{x})$$

or, in momentum space (and suppressing vector notation and spin indices)

$$\hat{V} = \frac{1}{2V^2} \iint \mathrm{d}\vec{x}\mathrm{d}\vec{y} \sum_{p_1,p_2,p_3,p_4} \mathrm{e}^{\mathrm{i}(-p_4 x - p_3 y + p_2 y + p_1 x)} a^{\dagger}_{p_4} a^{\dagger}_{p_3} v(x-y) a_{p_2} a_{p_1}\,.$$

Substituting $x \mapsto z = x - y$ ($x \mapsto z + y$), we get

$$\begin{aligned}\hat{V} &= \frac{1}{2} \sum_{p_1,p_2,p_3,p_4} a^{\dagger}_{p_4} a^{\dagger}_{p_3} a_{p_2} a_{p_1} \underbrace{\frac{1}{L}\int \mathrm{d}z\, v(z) \mathrm{e}^{-\mathrm{i}(p_1-p_4)z}}_{\widetilde{v}_{p_1-p_4}} \underbrace{\frac{1}{L}\int \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}(p_1+p_2-p_3-p_4)y}}_{\delta(p_4-(p_1+p_2-p_3))} \\ &= \frac{1}{2} \sum_{p_1,p_2,p_3} \widetilde{v}_{p_3-p_2} a^{\dagger}_{p_1+p_2-p_3} a^{\dagger}_{p_3} a_{p_2} a_{p_1}\,.\end{aligned}$$

Finally, we write $p_2 - p_3 = q$ (and hence $p_3 = p_2 - q$) and reinstate vector notation and spin indices to get

$$\hat{V} = \frac{1}{2} \sum_{\sigma_1,\sigma_2} \sum_{\vec{p}_1,\vec{p}_2,\vec{q}} \widetilde{v}_{\vec{q}}\, a^{\dagger}_{\vec{p}_1+\vec{q},\sigma_1} a^{\dagger}_{\vec{p}_2-\vec{q},\sigma_2} a_{\vec{p}_2,\sigma_2} a_{\vec{p}_1,\sigma_1}\,. \tag{11}$$

Equation (11) has a clear physical interpretation in terms of the Feynman diagram shown in figure. 1. A particle with in state $|\vec{p}_2, \sigma_2\rangle$ emits a force-carrying particle (e.g., a photon) with momentum $\vec{q}$ and ends up in a state $|\vec{p}_2 - \vec{q}, \sigma_2\rangle$. The force particle is absorbed by a particle initially in state $|\vec{p}_1, \sigma_1\rangle$ scattered to $|\vec{p}_1 + \vec{q}, \sigma_1\rangle$. The exchange of the force particle corresponds to an interaction between the two particles, described by the matrix element $\widetilde{v}_{\vec{q}}$ that conserves total momentum.

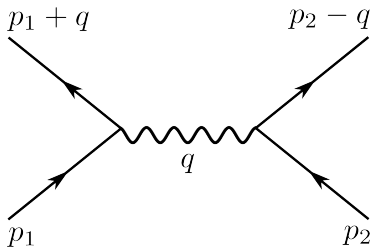


Figure 1: Illustration of the Coulomb interaction.

In solid-state physics, it is common to consider particles confined to the discrete set of unit cells (sites) of a crystal lattice. Similar to chapter 1, models are often written in terms of operators that create/destroy particles at a specific lattice site. For example, the Hubbard model describes electrons that hop between neighbouring lattice sites (kinetic energy, t is the so-called overlap or hopping integral) and experience a repulsive interaction if two electrons occupy the same site (a crude but useful approximation to the Coulomb repulsion). The model is defined by the Hamiltonian

$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} \,.$$

4.2 Coherent states for bosons and fermions

Since we can now write down models in terms of Hamiltonians using the language of second quantization, we need basis states to evaluate expectation values of the form $\langle \mathrm{e}^{-\beta \hat{H}} \rangle$. Following the idea of the path integral, we will discretize (imaginary) time and insert complete sets of eigenstates.

4.2.1 Coherent states for bosons

Boson coherent states for a single harmonic oscillator are constructed to be eigenstates of the annihilation operator a:

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

We expand a state $|\phi'\rangle$ in the occupation number basis, $|\phi'\rangle = \sum_{n=0}^{\infty} c_n\,|n\rangle$, so that the eigenvalue equation takes the form

$$a\,|\phi'\rangle = \sum_{n=0}^{\infty} c_n a\,|n\rangle = \sum_{n=1}^{\infty} c_n\sqrt{n}\,|n-1\rangle \stackrel{!}{=} \sum_{n=0}^{\infty} c_n\phi'\,|n\rangle$$

from which we obtain the condition on the coefficients $c_n = \phi' c_{n-1}/\sqrt{n} = c_0\phi'^n/\sqrt{n!}$. Consequently,

$$|\phi'\rangle = \sum_{n=0}^{\infty} c_n\,|n\rangle = \sum_{n=0}^{\infty} \frac{c_0\phi'^n}{\sqrt{n!}}\frac{(a^\dagger)^n}{\sqrt{n!}}\,|0\rangle = c_0\sum_{n=0}^{\infty}\frac{(\phi'\,a^\dagger)^n}{n!}\,|0\rangle = c_0\,\mathrm{e}^{\phi'\,a^\dagger}\,|0\rangle$$

and we can define (leaving out the prefactor c_0)

$$|\phi\rangle = \mathrm{e}^{\phi\,a^\dagger}\,|0\rangle$$

Hermitian conjugation gives

$$\langle\phi|\,a^\dagger = \langle\phi|\,\phi^*\,, \quad \langle\phi| = \langle 0|\,\mathrm{e}^{\phi^* a}\,.$$

The eigenvalues ϕ are complex numbers. The overlap of two coherent states is given by

$$\langle\psi\mid\phi\rangle = \langle 0|\,\mathrm{e}^{\psi^* a}\,|\phi\rangle = \langle 0|\,\mathrm{e}^{\psi^*\phi}\,|\phi\rangle = \mathrm{e}^{\psi^*\phi}\,\langle 0\mid\phi\rangle = \mathrm{e}^{\psi^*\phi}$$

and the norm (corresponding to the coefficient c_0 above) is

$$\langle\phi\mid\phi\rangle = \mathrm{e}^{\phi^*\phi}\,.$$

We can immediately generalize these results to more than one bosonic mode by defining

$$|\phi\rangle = \mathrm{e}^{\sum_i \phi_i a_i^\dagger}\,|0\rangle$$

with the properties

$$a_i \left|\phi\right\rangle = \phi_i \left|\phi\right\rangle \ , \quad \left\langle\psi \mid \phi\right\rangle = \mathrm{e}^{\sum_i \psi_i^* \phi_i} \ , \quad \left\langle\phi \mid \phi\right\rangle = \mathrm{e}^{\sum_i \phi_i^* \phi_i} \ .$$

The eigenvalues of the coherent states preserve the commutation relations of the bosonic operators $a_i, a_i^\dagger$,

$$[a_i, a_i^\dagger] \left|\phi\right\rangle = \delta_{ij} \left|\phi\right\rangle \ ,$$

and the coherent states form an (overcomplete) basis of states in Fock space,

$$\int \prod_i \frac{\mathrm{d}\phi_i^* \mathrm{d}\phi_i}{2\pi\mathrm{i}} \mathrm{e}^{-\sum_i \phi_i^* \phi_i} \left|\phi\right\rangle \left\langle\phi\right| = \hat{1} \, . \tag{12}$$

where $\frac{\mathrm{d}\phi_i^* \mathrm{d}\phi_i}{2\pi\mathrm{i}} = \frac{\mathrm{dRe}\,\phi_i \mathrm{dIm}\,\phi_i}{\pi}$. Equation (12) allows to write the trace of an operator in the form (introducing a complete basis $\{|\alpha\rangle\}$)

$$\begin{aligned}
\mathrm{Tr}\hat{A} &= \sum_\alpha \left\langle\alpha\right| \hat{A} \left|\alpha\right\rangle \\
&= \int \prod_i \frac{\mathrm{d}\phi_i^* \mathrm{d}\phi_i}{2\pi\mathrm{i}} \mathrm{e}^{-\sum_i \phi_i^* \phi_i} \sum_\alpha \left\langle\alpha \mid \phi\right\rangle \left\langle\phi\right| \hat{A} \left|\alpha\right\rangle \\
&= \int \prod_i \frac{\mathrm{d}\phi_i^* \mathrm{d}\phi_i}{2\pi\mathrm{i}} \mathrm{e}^{-\sum_i \phi_i^* \phi_i} \left\langle\phi\right| \hat{A} \sum_\alpha \left|\alpha\right\rangle \left\langle\alpha \mid \phi\right\rangle \\
&= \int \prod_i \frac{\mathrm{d}\phi_i^* \mathrm{d}\phi_i}{2\pi\mathrm{i}} \mathrm{e}^{-\sum_i \phi_i^* \phi_i} \left\langle\phi\right| \hat{A} \left|\phi\right\rangle
\end{aligned}$$

If the operator $\hat{A} = \hat{A}(a_i^\dagger, a_i)$ is normal-ordered (all $a^\dagger$'s left of all a 's), it is easy to evaluate matrix elements with respect to coherent states:

$$\left\langle\phi\right| \hat{A}(a_i^\dagger, a_i) \left|\phi'\right\rangle = A(\phi_i^*, \phi_i' \,) \, \mathrm{e}^{\sum_i \phi_i^* \phi_i'} \ = A(\phi_i^*, \phi_i' \,) \, \left\langle\phi \mid \phi'\right\rangle \ .$$

4.2.2 Coherent states for fermions

While for bosons the operators and coherent state eigenvalues commute,

$$a_i a_j \left|\phi\right\rangle = \phi_i \phi_j \left|\phi\right\rangle = \phi_j \phi_i \left|\phi\right\rangle = a_j a_i \left|\phi\right\rangle \quad \text{for} \quad i \neq j$$

we know that for fermions the commutation relations imply $a_i a_j = -a_j a_i$. Assuming that we can find eigenstates of fermionic annihilation operators, the eigenvalues would have to anticommute as well:

$$a_i \left|\eta\right\rangle = \eta_i \left|\eta\right\rangle \longrightarrow \eta_i \eta_j = -\eta_j \eta_i \,.$$

For $i = j$, we have $\eta_i \eta_i = \eta_i^2 = 0$ (Pauli principle). Because regular numbers do not have this property, it is necessary to introduce the algebra of Grassmann numbers. Any two Grassmann numbers anticommute,[23] and Grassmann numbers anticommute with operators a and $a^\dagger$. Grassmann numbers commute with regular real or complex numbers, and pairs of Grassmann variables (arising from, e.g., $a^\dagger a$) behave like bosonic objects: $\overline{\eta}\eta\overline{\theta}\theta = \overline{\theta}\theta\overline{\eta}\eta$.

Because of the property $\eta^2 = 0$, the Taylor expansion of $f(\eta)$ is simply[24]

$$f(\eta) = f_0 + f_1 \eta$$

while for a function of two variables η_1, η_2 we have

$$f(\eta_1, \eta_2) = f_0 + f_1\eta_1 + f_2\eta_2 + f_{12}\eta_1\eta_2 \,.$$

Differentiation is defined as for complex variables,

$$\frac{\partial}{\partial\eta}\eta = 1 \,, \quad \frac{\partial}{\partial\eta} a = 0 \,,$$

with the additional condition that the differential operator has to stand directly next to the variable it acts on:[25]

$$\frac{\partial}{\partial\eta_2}(\eta_1\eta_2) = -\frac{\partial}{\partial\eta_2}(\eta_2\eta_1) = -\eta_1 \,.$$

Integration over Grassmann variables is defined as

$$\int \mathrm{d}\eta\, \eta = 1 \,, \quad \int \mathrm{d}\eta\, 1 = 0 \,,$$

which can be motivated in several different ways. The first relation is a normalization. The second relation follows, for example, by requiring that

[23] $\{\eta_i, \eta_j\} = \{\overline{\eta}_i, \overline{\eta}_j\} = \{\overline{\eta}_i, \eta_j\} = \{\eta_i, \overline{\eta}_j\} = 0$.

[24] The fact that all series necessarily converge also avoids any problems in defining the a convergent path integral.

[25] One may also say that ∂_η itself anticommutes with Grassmann numbers.

$\int \mathrm{d}\eta f(\eta+\eta) = \int \mathrm{d}\eta f(\eta)$ [in analogy with regular variables where $\int_{-\infty}^{\infty} f(x+c) = \int_{-\infty}^{\infty} f(x)$]. The above definitions imply (exercises) that integration and differentiation are identical for Grassmann numbers, and hence very simple. As in the case of the derivative, $\mathrm{d}\eta$ has to stand next to the variable it acts on, which may give rise to minus signs from commuting variables.

A fermion coherent state for a single mode can be written as

$$|\eta\rangle = \mathrm{e}^{-\eta a^\dagger}|0\rangle = (1-\eta a^\dagger)|0\rangle = |0\rangle - \eta|1\rangle$$

and is indeed an eigenstate of the operator c since

$$a|\eta\rangle = a(|0\rangle - \eta|1\rangle) = -a\eta|1\rangle = \eta a|1\rangle = \eta|0\rangle$$

is equal to (we use $\eta^2 = 0$)

$$\eta|\eta\rangle = \eta(|0\rangle - \eta|1\rangle) = \eta|0\rangle \ .$$

A bra coherent state is given by

$$\langle\eta| = \langle 0|\,\mathrm{e}^{-a\overline{\eta}} = \langle 0| - \langle 1|\,\overline{\eta} = \langle 0| + \overline{\eta}\,\langle 1|$$

where (despite the notation) $\overline{\eta}$ and η are independent variables not related by complex conjugation, and the overlap between two coherent states is

$$\langle\eta\,|\,\phi\rangle = (\langle 0| + \overline{\eta}\,\langle 1|)(|0\rangle - \phi\,|1\rangle) = 1 + \overline{\eta}\phi = \mathrm{e}^{\overline{\eta}\phi}\,.$$

Generalizing these findings to the many-mode case, we arrive at

$$|\eta\rangle = \mathrm{e}^{-\sum_i \eta_i a_i^\dagger}|0\rangle \ , \quad a_i|\eta\rangle = \eta_i|\eta\rangle \quad \langle\eta| = \langle 0|\,\mathrm{e}^{-\sum_i a_i^\dagger \overline{\eta}_i}\,, \quad \langle\eta|\,a_i^\dagger = \langle\eta|\,\overline{\eta}_i$$

The overlap of two states becomes

$$\langle\eta\,|\,\phi\rangle = \mathrm{e}^{\sum_i \overline{\eta}_i\phi_i}\,.$$

Importantly for the formulation of the path integral, we also have

$$\int \prod_i \mathrm{d}\overline{\eta}_i \mathrm{d}\eta_i \mathrm{e}^{-\sum_i \overline{\eta}_i\eta_i}|\eta\rangle\langle\eta| = \hat{1}\,.$$

The trace of an operator can be written as

$$\begin{aligned}
\mathrm{Tr}\hat{A} &= \sum_{\alpha} \langle\alpha|\, \hat{A}\, |\alpha\rangle \\
&= \int \prod_i \mathrm{d}\overline{\eta}_i \mathrm{d}\eta_i \mathrm{e}^{-\sum_i \overline{\eta}_i \eta_i} \sum_{\alpha} \langle\alpha \,|\, \eta\rangle \, \langle\eta|\, \hat{A}\, |\alpha\rangle \\
&= \int \prod_i \mathrm{d}\overline{\eta}_i \mathrm{d}\eta_i \mathrm{e}^{-\sum_i \overline{\eta}_i \eta_i} \sum_{\alpha} \langle -\eta|\, \hat{A}\, |\alpha\rangle \, \langle\alpha \,|\, \eta\rangle \\
&= \int \prod_i \mathrm{d}\overline{\eta}_i \mathrm{d}\eta_i \mathrm{e}^{-\sum_i \overline{\eta}_i \eta_i} \, \langle -\eta|\, \hat{A}\, |\eta\rangle
\end{aligned}$$

where $\langle\alpha \,|\, \eta\rangle \, \langle\eta \,|\, \alpha'\rangle = \langle -\eta \,|\, \alpha'\rangle \, \langle\alpha \,|\, \eta\rangle$ because coherent states (and hence also scalar products with Fock states $|\alpha\rangle$) involve Grassmann variables. Matrix elements of normal-ordered operators are simple to evaluate:

$$\langle\eta|\, \hat{A}(a_i^\dagger, a_i)\, |\eta'\rangle = A(\overline{\eta}_i, \eta_i') \, \mathrm{e}^{\sum_i \overline{\eta}_i \eta'} = A(\overline{\eta}_i, \eta_i') \, \langle\eta \,|\, \eta'\rangle \ .$$

4.2.3 Gaussian integrals

In the bosonic case, the use of coherent states leads to Gaussian integrals over pairs of complex conjugate variables, see also page 36. The relevant integral formula for N-dimensional complex vectors is

$$\int \prod_{i=1}^{N} \mathrm{d}v_i^* \mathrm{d}v_i \ \mathrm{e}^{-\sum_{ij} v_i^* A_{ij} v_j + \sum_i w_i^* v_i + \sum_i v_i^* w_i'} = \pi^N \det A^{-1} \, \mathrm{e}^{\sum_{ij} w_i^* A_{ij}^{-1} w_j'} \ .$$

For Gaussian Grassmann integrals, it can be shown that[26]

$$\int \prod_{i=1}^{N} \mathrm{d}\overline{\eta}_i \mathrm{d}\eta_i \, \mathrm{e}^{-\sum_{ij} \overline{\eta}_i A_{ij} \eta_j + \sum_i \overline{\xi}_i \eta_i + \sum_i \xi_i \overline{\eta}_i} = \det A \, \mathrm{e}^{\sum_{ij} \overline{\xi}_i A_{ij}^{-1} \xi_j} \ .$$

Hence, the determinant appears in the numerator rather than the denominator, and the factor π^N is absent.

[26] $\overline{\xi}$ and ξ are independent Grassmann variables.

4.3 Quantum partition function as a field integral

Equipped with our knowledge about second quantization and coherent states, we can formulate the partition function of many-particle quantum systems in terms of the path integral.

The grand canonical partition function is defined as

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

where μ is the chemical potential, $\hat{N}$ is the total particle number operator, and $\{|n\rangle\}$ is a complete set of many-particle Fock states. Writing the coherent state resolution of the identity operator as

$$\int \mathrm{d}(\overline{\psi}, \psi) \, \mathrm{e}^{-\sum_i \overline{\psi}_i \psi_i} \, |\psi\rangle \, \langle\psi| = \hat{1} \, . \tag{13}$$

where

$$\mathrm{d}(\overline{\psi}, \psi) = \prod_i \frac{\mathrm{d}\overline{\psi}_i \mathrm{d}\psi_i}{(2\pi\mathrm{i})^{(1+\zeta)/2}} = \begin{cases} \prod_i \frac{\mathrm{d}\psi_i^* \mathrm{d}\psi_i}{2\pi\mathrm{i}} & \text{bosons } (\zeta = +1) \\ \prod_i \mathrm{d}\overline{\psi}_i \mathrm{d}\psi_i & \text{fermions } (\zeta = -1) \end{cases} \ . \tag{14}$$

we can write the partition function as

$$\begin{aligned} Z &= \int \mathrm{d}(\overline{\psi}, \psi) \, \mathrm{e}^{-\sum_i \overline{\psi}_i \psi_i} \sum_n \langle n \mid \psi\rangle \, \langle\psi| \, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} \, |n\rangle \\ &= \int \mathrm{d}(\overline{\psi}, \psi) \, \mathrm{e}^{-\sum_i \overline{\psi}_i \psi_i} \, \langle\zeta\psi| \, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} \, |\psi\rangle \ , \end{aligned} \tag{15}$$

To proceed, we assume a generic Hamiltonian with of the form

$$\hat{H} = \sum_{ij} h_{ij} a_i^\dagger a_j + \sum_{ijpq} V_{ijpq} a_i^\dagger a_j^\dagger a_p a_q \, . \tag{16}$$

A Trotter expansion of the exponential, $\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} \approx \prod_{k=1}^N \mathrm{e}^{-\Delta\tau(\hat{H}-\mu\hat{N})}$ (with $\Delta\tau = \beta/N$) and the insertion of unity [equation (13)] on each time slice gives

$$\langle\zeta\psi| \, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} \, |\psi\rangle = \int \prod_{k=1}^{N-1} \mathrm{d}(\overline{\psi}_k, \psi_k) \, \mathrm{e}^{-\sum_i \overline{\psi}_{i,k} \psi_{i,k}} \prod_{k=1}^{N} \langle\psi_k| \, \mathrm{e}^{-\Delta\tau(\hat{H}-\mu\hat{N})} \, |\psi_{k-1}\rangle$$

with the conditions $\overline{\psi}_N = \zeta\overline{\psi}$ and $\psi_0 = \psi$.[27] We can calculate $\langle\psi_k|\,\hat{A}(a_i^\dagger, a_i)\,|\psi_{k-1}\rangle$ by replacing operators with their eigenvalues.[28] We have

$$\langle\psi_k|\,\mathrm{e}^{-\Delta\tau[\hat{H}-\mu\hat{N}]}\,|\psi_{k-1}\rangle = \mathrm{e}^{-\Delta\tau[H(\overline{\psi}_k,\psi_{k-1})-\mu N(\overline{\psi}_k,\psi_{k-1})]}\,\langle\psi_k\,|\,\psi_{k-1}\rangle$$

with

$$\begin{aligned} H(\overline{\psi}_k,\psi_{k-1}) &= \sum_{ij} h_{ij}\overline{\psi}_{i,k}\psi_{j,k-1} + \sum_{ijpq} V_{ijpq}\overline{\psi}_{i,k}\overline{\psi}_{j,k}\psi_{p,k-1}\psi_{q,k-1}\,, \\ N(\overline{\psi}_k,\psi_{k-1}) &= \sum_i \overline{\psi}_{i,k}\psi_{i,k-1}\,, \end{aligned}$$

and hence get

$$\begin{aligned} \prod_{k=1}^N \langle\psi_k|\,\mathrm{e}^{-\Delta\tau(\hat{H}-\mu\hat{N})}\,|\psi_{k-1}\rangle &= \prod_{k=1}^N \mathrm{e}^{-\Delta\tau[H(\overline{\psi}_k,\psi_{k-1})-\mu N(\overline{\psi}_k,\psi_{k-1})]}\,\langle\psi_k\,|\,\psi_{k-1}\rangle \\ &= \mathrm{e}^{-\Delta\tau\sum_{k=1}^N[H(\overline{\psi}_k,\psi_{k-1})-\mu N(\overline{\psi}_k,\psi_{k-1})]}\mathrm{e}^{\sum_{k=1}^N\overline{\psi}_k\psi_{k-1}} \end{aligned}$$

Returning to equation (15) and absorbing the additional integral over $\mathrm{d}(\overline{\psi},\psi) \equiv \mathrm{d}(\overline{\psi}_N,\psi_0)$ [with the boundary conditions $\overline{\psi}_0 = \zeta\overline{\psi}_N$, $\psi_0 = \zeta\psi_N$, cf. equation (15)] we obtain the discrete-time approximation

$$Z_N = \int \prod_{k=1}^N \mathrm{d}(\overline{\psi}_k,\psi_k)\,\mathrm{e}^{-S[\overline{\psi},\psi]}$$

with the action

$$S[\overline{\psi},\psi] = \Delta\tau\left[\sum_{k=1}^N \frac{\overline{\psi}_k(\psi_k-\psi_{k-1})}{\Delta\tau} + \sum_{k=1}^N [H(\overline{\psi}_k,\psi_{k-1}) - \mu N(\overline{\psi}_k,\psi_{k-1})]\right].$$

As before, we can formally take the continuum limit $N\to\infty$ to get

$$Z = \int\limits_{\substack{\overline{\psi}(0)=\zeta\overline{\psi}(\beta)\\ \psi(0)=\zeta\psi(\beta)}} \mathcal{D}[\overline{\psi},\psi]\,\mathrm{e}^{-S[\overline{\psi},\psi]}\,, \quad S[\overline{\psi},\psi] = \int_0^\beta \mathrm{d}\tau\,\left[\overline{\psi}\partial_\tau\psi + H(\overline{\psi},\psi) - \mu N(\overline{\psi},\psi)\right].$$

[27] The fields now have two indices: i refers to the orbitals/modes, and k to the time slice. To keep the notation simple, we suppress i when it does not lead to confusion.

[28] The Trotter discretization permits us to normal-order the exponential and neglect the error, $\mathrm{e}^{-\Delta\tau\hat{H}(a^\dagger,a)} =: \mathrm{e}^{-\Delta\tau\hat{H}(a^\dagger,a)} : +\mathcal{O}(\Delta\tau^2)$.

This form is valid for both fermions ($\zeta = -1$) and bosons ($\zeta = +1$) if we choose the corresponding integration variables [cf. equation (14)]. In this limit, we have a functional integral over coherent state variables (eigenvalues, either complex numbers of Grassmann numbers) $\overline{\psi}_i(\tau), \psi_i(\tau)$ that are functions of imaginary time τ.

For a Hamiltonian of the form (16), the action can be written as

$$S[\overline{\psi}, \psi] = \int_0^\beta \mathrm{d}\tau \left[\sum_{ij} \overline{\psi}_i(\tau)[(\partial_\tau - \mu)\delta_{ij} + h_{ij}]\psi_j(\tau) + \sum_{ijpq} V_{ijpq}\overline{\psi}_i(\tau)\overline{\psi}_j(\tau)\psi_p(\tau)\psi_q(\tau) \right] .$$

Alternatively, the action S may also be regarded as the time-integral of a Lagrangian, $S = \int \mathrm{d}\tau \mathcal{L}_\mathrm{E}$, where $\mathcal{L}_\mathrm{E}$ could for example correspond to the non-relativistic complex field theory with $\mathcal{L}_\mathrm{E} = \psi^\dagger \partial_\tau \psi + \frac{1}{2m}\nabla\psi^\dagger \cdot \nabla\psi$, cf. chapter 2.3. For a simple real field theory, we have $Z = \int \mathcal{D}[\phi]\, \mathrm{e}^{-S[\phi]}$.

Instead of the imaginary-time representation, the field integral is often used in the Matsubara-frequency representation. The representations are linked by the Fourier transforms

$$\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \psi_n \, \mathrm{e}^{-\mathrm{i}\omega_n \tau} , \quad \psi_n = \frac{1}{\sqrt{\beta}} \int_0^\beta \mathrm{d}\tau \, \psi(\tau) \, \mathrm{e}^{\mathrm{i}\omega_n \tau}$$

where the (anti-)periodicity of the fields with period β gives rise to the Matsubara frequencies ($n \in \mathbb{Z}$)

$$\omega_n = \begin{cases} 2n\pi/\beta & \text{bosons} \\ (2n+1)\pi/\beta & \text{fermions} \end{cases}$$

and the action becomes

$$S[\overline{\psi}, \psi] = \sum_{\substack{ij \\ n}} \overline{\psi}_{i,n}[(-\mathrm{i}\omega_n - \mu)\delta_{ij} + h_{ij}]\psi_{j,n} + \frac{1}{\beta} \sum_{\substack{ijpq \\ n_1 n_2 n_3 n_4}} V_{ijpq}\overline{\psi}_{i,n_1}\overline{\psi}_{j,n_2}\psi_{p,n_3}\psi_{q,n_4}\delta_{n_1+n_2+n_3+n_4} .$$

Let us calculate Z for free particles in one dimension, for which the Hamiltonian is diagonal in momentum space, $\hat{H}_0 = \sum_p \epsilon_p a_p^\dagger a_p$. The easiest way to do so is to resort to the discrete path integral and then take the limit $N \to \infty$. Because $\hat{H}_0$ is diagonal, the partition function factorizes, $Z_N = \prod_p Z_N^{(p)}$, with

$$\begin{aligned} Z_N^{(p)} &= \int \prod_{k=1}^{N} \mathrm{d}(\overline{\psi}_k, \psi_k) \, \exp\left[-\sum_{k=1}^{N} \left\{ \overline{\psi}_k(\psi_k - \psi_{k-1}) - \Delta\tau \overline{\psi}_k \psi_{k-1}(\epsilon_p - \mu) \right\} \right] \\ &= \int \prod_{k=1}^{N} \mathrm{d}(\overline{\psi}_k, \psi_k) \, \exp\left[-\sum_{k=1}^{N} \left\{ \overline{\psi}_k \psi_k + \overline{\psi}_k(1 - \Delta\tau(\epsilon_p - \mu))\psi_{k-1} \right\} \right] . \end{aligned}$$

The action can be written in the form $-[\vec{\overline{\psi}}]^T S^{(p)} \vec{\psi}$ with the $N \times N$ matrix

$$S^{(p)} = \begin{pmatrix} 1 & 0 & & \cdots & 0 & -\zeta a \\ -a & 1 & 0 & & & 0 \\ 0 & -a & 1 & \ddots & & \vdots \\ \vdots & & 0 & -a & 1 & 0 \\ 0 & & & \cdots & -a & 1 \end{pmatrix}$$

where $a = 1 - \Delta\tau(\epsilon_p - \mu)$ and the top right element accounts for the boundary conditions on the fields. Gaussian integration gives[29][30]

$$Z_0 = \lim_{N\to\infty} \prod_p Z_N^{(p)} = \lim_{N\to\infty} \prod_p [\det S^{(p)}]^{-\zeta} .$$

The determinant can be calculated by expanding along the first row

$$\begin{aligned} \lim_{N\to\infty} [\det S^{(p)}] &= \lim_{N\to\infty} \left[1 D_{11} - (-1)^N (-\zeta a) D_{1N}) \right] \\ &= \lim_{N\to\infty} \left[1 - (-1)^N (-\zeta a)(-a)^{N-1} \right] \\ &= 1 - \zeta \lim_{N\to\infty} \left(1 - \frac{\beta(\epsilon_p - \mu)}{N} \right)^N = 1 - \eta \mathrm{e}^{-\beta(\epsilon_p - \mu)} \end{aligned}$$

and the partition function is therefore as expected

$$Z_0 = \prod_p \left(1 - \zeta \mathrm{e}^{-\beta(\epsilon_p - \mu)} \right)^{-\zeta} .$$

[29] The measure in equation (14) ensures that the factor π^N is cancelled in the bosonic case.

[30] The partition function of a quadratic (Gaussian) theory is essentially $[\det \hat{D}]^{-\zeta}$.

4.4 Generating functional and response functions

While the partition function is sufficient to calculate important thermodynamic properties such as the energy ($\langle E\rangle = -\partial \ln Z/\partial\beta$) or the specific heat ($c_V = \partial\langle E\rangle/\partial T$), we were reminded in chapter 3.8 that correlation functions are best calculated from a generating function(al). In fact, the latter contains everything that can be known about a quantum field theory (or the corresponding Hamiltonian), making it the key object of interest.

In the field theory context, the need to consider a generating functional with source fields is motivated by the fact that the fields are not physically observable. As a consequence, transition amplitudes between eigenstates (e.g., $\langle q_b, t_b \,|\, q_a, t_a\rangle$, as considered in the single-particle case) are not of interest. Adding source terms allows to measure the correlations between fields that are experimentally accessible (see below). Here, we first define the generating functional and then illustrate how correlation functions between fields are related to physical expectation values.

4.4.1 Generating functional

We consider a noninteracting real scalar field theory with action $S = \int \mathrm{d}^4x \mathcal{L}_\mathrm{E}$ and Lagrange density (the potential has a plus sign in imaginary time)[31]

$$\mathcal{L}_\mathrm{E} = \tfrac{1}{2}(\partial_\mu\phi)^2 + \tfrac{1}{2}m^2\phi^2 = \tfrac{1}{2}(\partial_\tau\phi)^2 + \tfrac{1}{2}(\nabla\phi)^2 + \tfrac{1}{2}m^2\phi^2$$

and disturb it by adding $-J(x)\phi(x)$ to define the functional[32][33]

$$Z[J] = \int \mathcal{D}[\phi]\mathrm{e}^{-S+\int \mathrm{d}^4x J\phi}$$

which reduces to the partition function for $J = 0$, i.e., $Z = Z[0]$. The generating functional permits us to calculate expectation values of fields via differentiation. Defining the expectation value of $A(\phi)$ as

$$\langle A\rangle = \frac{\int \mathcal{D}[\phi]\mathrm{e}^{-S[\phi]}A(\phi)}{\int \mathcal{D}[\phi]\mathrm{e}^{-S[\phi]}} = \frac{1}{Z}\int \mathcal{D}[\phi]\mathrm{e}^{-S[\phi]}A(\phi)$$

[31] For $\phi(x) = \phi(\tau)$ (zero spatial dimensions) this corresponds to the harmonic oscillator.
[32] The symbol Z implies (anti-)periodic boundary conditions for bosons (fermions).
[33] For a complex field theory, a suitable source term would be $-J\psi^* - J^*\psi$.

the functional derivative with respect to the source gives

$$\frac{1}{Z[0]}\frac{\delta Z[J]}{\delta J(x_1)}\bigg|_{J=0} = \frac{\int \mathcal{D}[\phi]\mathrm{e}^{-S}\phi(x_1)}{\int \mathcal{D}[\phi]\mathrm{e}^{-S[\phi]}} = \langle\phi(x_1)\rangle\,.$$

Similarly, the correlation function $\langle\phi(x_1)\phi(x_2)\rangle$ can be obtained from

$$\langle\phi(x_1)\phi(x_2)\rangle = \frac{\int \mathcal{D}[\phi]\mathrm{e}^{-S}\phi(x_1)\phi(x_2)}{\int \mathcal{D}[\phi]\mathrm{e}^{-S[\phi]}} = \frac{1}{Z[0]}\frac{\delta^2 Z[J]}{\delta J(x_1)\delta J(x_2)}\bigg|_{J=0}\,.$$

For Gaussian theories, the functional integral and hence $Z[J]$ and all the correlation functions can be calculated exactly. For our example,

$$Z[J] = \int \mathcal{D}[\phi]\mathrm{e}^{-\frac{1}{2}\int \mathrm{d}^4x\,\phi[\partial_\mu^2+m^2]\phi+\int \mathrm{d}^4x\,J\phi} = Z[0]\,\mathrm{e}^{\iint \mathrm{d}^4x\mathrm{d}^4y J(x)D(x-y)J(y)}$$

where $D(x-y)$ is the Green function of the operator $[\partial_\mu^2+m^2]$ and describes how the field propagates between the points x and y where the perturbations $J(x)$ and $J(y)$ take place. Taking the second functional derivative of $Z[J]/Z[0]$ gives the result $\langle\phi(x)\phi(y)\rangle = D(x-y)$, and the correlation function $\langle\phi(x)\phi(y)\rangle$ is therefore called the Green function, propagator, or two-point function. For the present case, the momentum-space and Matsubara-frequency representation is given by $D(\vec{p},\mathrm{i}\omega_n) = [\omega_n^2+|\vec{p}|^2+m^2]^{-1}$.

4.4.2 Relation to response functions

Much of the understanding of materials comes from experiments that measure the response to external perturbations such as voltages, thermal gradients, or electromagnetic radiation. It is therefore of particular importance to be able to calculate the response for a given model theoretically.

Consider an experiment in which a time-dependent perturbation (or generalized force) $J(\vec{r},t)$ couples to an operator $\hat{A}$, as described by a term

$$\hat{H}_J(t) = \int \mathrm{d}^d r J(\vec{r},t)\hat{A}(\vec{r})\,.$$

in the Hamiltonian. For example, $J(\vec{r},t)$ could be an electric voltage $\phi(\vec{r},t)$ and $\hat{A}$ the charge density operator $\hat{\rho}$. We assume that $\hat{H}_J(t)$ is a small

perturbation that leads to a time-dependent expectation value $B(\vec{r},t)$ of an observable $\hat{B}$. To linear order in the perturbation (*linear response*), we expect

$$B(\vec{r},t) \sim \int \mathrm{d}^d r' \int \mathrm{d}t' \chi(\vec{r},t,\vec{r}',t') J(\vec{r}',t') \,. \tag{17}$$

The quantity $\chi(\vec{r},t,\vec{r}',t')$ gives the functional relation between a perturbation J coupling to $\hat{A}$ and the resulting change of $\langle \hat{B} \rangle$. It is called a response function or susceptibility. For scalar quantities $\hat{A}, \hat{B}, J$ χ is just a function, but in general it will be a tensor χ_{ij}. For example, the conductivity tensor has longitudinal (σ_{xx}) and Hall components (σ_{xy}).

We can deduce several properties of χ based on physical principles. Causality implies that B cannot change before the perturbation J starts, so $\chi = 0$ for $t < t'$ (retarded response). If the original Hamiltonian (without $\hat{H}_J$) is independent of time, χ will depend only on $t - t'$. Fourier transformation then leads to the relation

$$B(\vec{r},\omega) \sim \int \mathrm{d}^d r' \chi(\vec{r},\vec{r}',\omega) J(\vec{r}',\omega) \,,$$

which implies that a perturbation with frequency ω will lead to a response of the system with the same frequency (within the linear approximation). Similarly, if we have translation invariance, χ will depend on $\vec{r} - \vec{r}'$ and we can Fourier transform to momentum space to obtain

$$B(\vec{q},\omega) = \chi(\vec{q},\omega) J(\vec{q},\omega) \,.$$

To derive an expression for the response function that can be calculated using the path-integral method, we assume that $\hat{A}$ and $\hat{B}$ are scalar single-particle operators and can therefore be written as $\hat{A} = \sum_{mn} A_{mn} a_m^\dagger a_n$ and $\hat{B} = \sum_{mn} B_{mn} a_m^\dagger a_n$. The path-integral expectation value of $\hat{B}$ (in imaginary time) takes the form[34]

$$\langle \hat{B} \rangle = B(\tau) = \sum_{mn} B_{mn} \langle \overline{\psi}_m(\tau) \psi_n(\tau) \rangle$$

and is taken with respect to the action $S[\overline{\psi},\psi,J] = S_0[\overline{\psi},\psi] + \delta S^A_{J'}[\overline{\psi},\psi,J']$ with the perturbation

$$\delta S^A_{J'}[\overline{\psi},\psi,J'] = \int \mathrm{d}\tau \, H_{J'}(\overline{\psi},\psi) = \int \mathrm{d}\tau J'(\tau) \sum_{mn} A_{mn} \overline{\psi}_m(\tau) \psi_n(\tau) \,.$$

[34] For simplicity, we only keep track of the time dependence of the expectation value.

We assume $B(\tau) = 0$ for $J' = 0$. The expectation value can be written as the derivative of a suitable generating functional,[35]

$$B(\tau) = -\left.\frac{1}{Z[0,J']}\frac{\delta Z[J,J']}{\delta J}\right|_{J=0} = -\left.\frac{\delta}{\delta J}\right|_{J=0} \ln Z[J,J']$$

where we added a second perturbation (or source term) coupling to $\hat{B}$ via

$$\delta S_J^B[\overline{\psi},\psi,J] = \int \mathrm{d}\tau J(\tau) \sum_{mn} B_{mn}\overline{\psi}_m(\tau)\psi_n(\tau)\,.$$

to get $S = S_0 + \delta S_{J'}^A + \delta S_J^B$ and

$$Z[J,J'] = \int \mathcal{D}[\overline{\psi},\psi]\mathrm{e}^{-S[\overline{\psi},\psi,J,J']}\,.$$

$Z[0,J']$ is the partition function of the system with perturbation $H_{J'}$. $Z[J,J']$ is a generating functional with an additional source term that couples J to B and allows us to calculate the expectation value $B(\tau)$.

Assuming the physical perturbation J' to be weak, we consider $\ln Z[J,J']$ as a functional $G[J']$ that we expand to linear order in J' to obtain[36]

$$B(\tau) \approx -\int \mathrm{d}\tau' \left.\frac{\delta^2}{\delta J(\tau)\delta J'(\tau')}\right|_{J,J'=0} \ln Z[J,J']J'(\tau')\,.$$

Comparison with equation (17) suggests that

$$\chi(\tau,\tau') = -\left.\frac{\delta^2}{\delta J(\tau)\delta J'(\tau')}\ln Z[J,J']\right|_{J,J'=0} = -\frac{1}{Z}\left.\frac{\delta^2 Z[J,J']}{\delta J(\tau)\delta J'(\tau')}\right|_{J,J'=0}\,.$$

On the other hand, we know from the previous section that the second derivative of a generating functional corresponds to a correlation function. In the present case, the response function involves a four-point function:

$$\chi(\tau,\tau') = -\langle\hat{B}(\tau)\hat{A}(\tau')\rangle = -\sum_{mn}\sum_{pq} B_{mn}A_{pq}\,\langle\overline{\psi}_m(\tau)\psi_n(\tau)\overline{\psi}_p(\tau')\psi_q(\tau')\rangle\,.$$

[35] We defined the perturbation with as $+\int JA$, and get an overall $-$ from the derivative.
[36] See footnote on page 53.

For example, a magnetic field coupling to spins via $\hat{H}_J = \int \mathrm{d}^d r\, J\hat{S}^z$ will change the expectation value of spin operators (the magnetization), as described by the magnetic susceptibility $\chi^{zz} \sim \langle S^z(\tau) S^z(\tau')\rangle$. Similarly, the nontrivial (interacting) contribution to the electric conductivity is determined by the current-current correlation function. The path integral gives correlation functions in imaginary time τ or for Matsubara frequencies $\mathrm{i}\omega_n$. A comparison with experiment requires continuation to real time/frequencies.

Finally, the generating functional for a Hamiltonian system in the coherent state representation takes the form

$$Z[J, \overline{J}] = \int \mathcal{D}[\overline{\psi}, \psi]\, \mathrm{e}^{-S[\overline{\psi},\psi]+\langle\overline{\psi}J\rangle+\langle\overline{J}\psi\rangle}\,,$$

where $\langle a, b\rangle$ is a short-hand for the scalar product $\sum_i \int \mathrm{d}\tau a_i(\tau) b_i(\tau)$.

4.4.3 Relation to expectation values of operators

We know now how to calculate field expectation values $\langle\phi(x_1)\phi(x_2)\rangle$ from a generating functional, and that such correlation functions are related to experimentally accessible response functions. A final but important detail is how exactly expressions like $\langle\phi(x_1)\phi(x_2)\rangle$ are related to expectation values of operators $\hat{\phi}$. To this end, we briefly return to the single-particle path integral, and consider the expression

$$\int \mathcal{D}[q(t)]\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_0^T \mathrm{d}tL}\, q(t_1)\,.$$

Returning to the derivation in discrete time, we can regard $q(t_1)$ as the eigenvalue of the position operator $\hat{q}$ evaluated on the time-slice where $n_1\Delta t = t_1$:

$$\langle q_b|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\Delta t\hat{H}}\, |q_{N-1}\rangle \ldots \langle q_{n_1+1}|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\Delta t\hat{H}}\, q(t_1)\, |q_{n_1}\rangle \ldots \langle q_1|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\Delta t\hat{H}}\, |q_a\rangle\ .$$

Replacing $\langle q_{n_1+1}|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\Delta t\hat{H}}\, q(t_1)\, |q_{n_1}\rangle$ with $\langle q_{n_1+1}|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\Delta t\hat{H}}\hat{q}\, |q_{n_1}\rangle$ and returning to the continuum limit suggests that

$$\int \mathcal{D}[q(t)]\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_0^T \mathrm{d}tL}\, q(t_1) = \langle q_b|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(T-t_1)}\, \hat{q}\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t_1}\, |q_a\rangle = \langle q_b|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}T}\, \hat{q}_{\mathrm{H}}(t_1)\, |q_a\rangle\ .$$

where we invoked the Heisenberg representation $\hat{A}_{\mathrm{H}}(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{A}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}$.

In a second step, let us consider the path integral

$$\int \mathcal{D}[q(t)]\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_0^T \mathrm{d}tL}\, q(t_1)q(t_2)\,.$$

where we can again consider $q(t_1)$ and $q(t_2)$ as eigenvalues of $\hat{q}$ evaluated at times t_1 and t_2. However, an important point is that time increases from $t = 0$ to $t = T$ from right to left in the path integral, so that for $t_2 > t_1$

$$\begin{aligned}\int \mathcal{D}[q(t)]\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_0^T \mathrm{d}tL}\, q(t_1)q(t_2) &= \langle q_b|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(T-t_2)}\, \hat{q}\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t_2-t_1)}\, \hat{q}\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t_1}\, |q_a\rangle \\ &= \langle q_b|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}T}\, \hat{q}_{\mathrm{H}}(t_2)\hat{q}_{\mathrm{H}}(t_1)\, |q_a\rangle\end{aligned}$$

whereas for $t_2 < t_1$

$$\int \mathcal{D}[q(t)]\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_0^T \mathrm{d}tL}\, q(t_1)q(t_2) = \langle q_b|\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}T}\, \hat{q}_{\mathrm{H}}(t_1)\hat{q}_{\mathrm{H}}(t_2)\, |q_a\rangle\ .$$

The path integral gives us a time-ordered expectation value of operators:

$$\int \mathcal{D}[q(t)]\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_0^T \mathrm{d}tL}\, q(t_1)q(t_2) = \langle q(t_1)q(t_2)\rangle = \langle T[\hat{q}_{\mathrm{H}}(t_1)\hat{q}_{\mathrm{H}}(t_2)]\rangle\,,$$

with the time-ordering symbol defined as

$$T[\hat{q}_{\mathrm{H}}(t_1)\hat{q}_{\mathrm{H}}(t_2)] = \theta(t_1 - t_2)\hat{q}_{\mathrm{H}}(t_1)\hat{q}_{\mathrm{H}}(t_2) + \theta(t_2 - t_1)\hat{q}_{\mathrm{H}}(t_2)\hat{q}_{\mathrm{H}}(t_1)\,.$$

We can immediately extend these considerations to the functional integral in imaginary time. To this end, we consider second-quantized operators $\hat{A}[a^\dagger, a]$ and $\hat{B}[a^\dagger, a]$ and the imaginary-time Heisenberg representation $\hat{O}_{\mathrm{H}}(\tau) = \mathrm{e}^{\tau(\hat{H}-\mu\hat{N})}\hat{O}\mathrm{e}^{-\tau(\hat{H}-\mu\hat{N})}$. Defining the time-ordering operator as

$$T[\hat{A}_{\mathrm{H}}(\tau_1)\hat{B}_{\mathrm{H}}(\tau_2)] = \theta(\tau_1 - \tau_2)\hat{A}_{\mathrm{H}}(\tau_1)\hat{B}_{\mathrm{H}}(\tau_2) + \zeta_{AB}\theta(\tau_2 - \tau_1)\hat{B}_{\mathrm{H}}(\tau_2)\hat{A}_{\mathrm{H}}(\tau_1)$$

where $\zeta_{AB} = 1$ (-1) for bosonic (fermionic) operators, we have

$$\begin{aligned}\langle A(\tau_1)B(\tau_2)\rangle &= \frac{1}{Z}\int \mathcal{D}[\overline{\phi}, \phi]\, \mathrm{e}^{-S}\, A[\overline{\phi}(\tau_1), \phi(\tau_1)]B[\overline{\phi}(\tau_2), \phi(\tau_2)] \\ &= \frac{1}{Z}\mathrm{Tr}\left(T[\hat{A}_{\mathrm{H}}(\tau_1)\hat{B}_{\mathrm{H}}(\tau_2)]\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}\right) \\ &= \langle T[\hat{A}_{\mathrm{H}}(\tau_1)\hat{B}_{\mathrm{H}}(\tau_2)]\rangle\,.\end{aligned}$$

Note that in the path-integral formalism, the eigenvalues $\overline{\phi}, \phi$ are complex or Grassmann numbers but have no equal-time commutation relations, in contrast to the Heisenberg operators in the canonical formalism. For bosons, we may freely change the ordering of the eigenvalues, whereas for fermions the interchange of two Grassmann variables gives a minus sign. The latter is reflected in the definition of the time-ordering symbol T.[37] Reordering of A and B in the path-integral expectation value $\langle A(\tau_1)B(\tau_2)\rangle$ can only change the sign. Therefore, $\langle A(\tau_1)B(\tau_2)\rangle$ cannot correspond to $\langle \hat{A}_{\mathrm{H}}(\tau_1)\hat{B}_{\mathrm{H}}(\tau_2)\rangle$ because changing the order in which operators act on the states usually gives completely different results. Instead, $\langle A(\tau_1)B(\tau_2)\rangle$ has to correspond to something that is (up to a sign) independent of the operator order, namely the time-ordered expectation value $\langle T[\hat{A}_{\mathrm{H}}(\tau_1)\hat{B}_{\mathrm{H}}(\tau_2)]\rangle$.

The above observations suggest that the key objects of interest will have the form of so-called Matsubara Green functions defined as

$$G_{AB}(\tau_1,\tau_2) = -\langle T[\hat{A}_{\mathrm{H}}(\tau_1)\hat{B}_{\mathrm{H}}(\tau_2)]\rangle\,.$$

The simplest case are propagators $-\langle T[a_{\mathrm{H}}(\tau_1)a^{\dagger}_{\mathrm{H}}(\tau_2)]\rangle$ (also called single-particle Green functions) given by expectation values of the form $\langle\phi(\tau_1)\overline{\phi}(\tau_2)\rangle$.

4.5 Perturbation theory

We have seen above that for Gaussian problems we can calculate the generating functional exactly and thereby obtain any correlation functions or expectation values of interest. Unfortunately, most interesting problems are not of the Gaussian form. Consider the 1D generating function

$$Z_\lambda(J) = \int \mathrm{d}\phi\, \mathrm{e}^{-\frac{1}{2}a\phi^2+\lambda\phi^4+J\phi}\,.$$

The term $V(\phi) = \lambda\phi^4$ (the interaction term of ϕ^4 theory) makes the integral non-Gaussian. However, we can rewrite the integral as

$$Z_\lambda(J) = \int \mathrm{d}\phi\, \mathrm{e}^{-\frac{1}{2}a\phi^2+J\phi}\mathrm{e}^{\lambda\phi^4}$$

[37] Therefore, $T[\hat{A}(\tau_1)\hat{B}(\tau_2)] = \zeta T[\hat{B}(\tau_2)\hat{A}(\tau_1)]$.

and expand $\mathrm{e}^{\lambda\phi^4}$ in powers of the interaction strength λ to get

$$Z_\lambda(J) = \int \mathrm{d}\phi\, \mathrm{e}^{-\frac{1}{2}a\phi^2+J\phi} \left(1 + \lambda\phi^4 + \frac{(\lambda\phi^4)^2}{2!} + \frac{(\lambda\phi^4)^3}{3!} + \dots\right) .$$

With the free generating function $Z_0(J) = \int \mathrm{d}\phi\, \mathrm{e}^{-\frac{1}{2}a\phi^2+J\phi}$ we have

$$\frac{Z_\lambda(J)}{Z_0(J)} = \left[1 + \lambda\langle\phi^4\rangle_0^J + \frac{\lambda^2}{2!}\langle\phi^8\rangle_0^J + \frac{\lambda^3}{3!}\langle\phi^{12}\rangle_0^J + \dots\right]$$

where the expectation values are with respect to the non-interacting theory,

$$\langle A\rangle_0^J = \frac{1}{Z_0(J)} \int \mathrm{d}\phi\, \mathrm{e}^{-\frac{1}{2}a\phi^2+J\phi} A\,.$$

The series expansion can also be written as

$$Z_\lambda(J) = \left[1 + \lambda\left(\frac{\partial}{\partial J}\right)^4 + \frac{\lambda^2}{2!}\left(\frac{\partial}{\partial J}\right)^8 + \dots\right] Z_0(J) = Z_0(0)\, \mathrm{e}^{\lambda(\partial/\partial J)^4}\, \mathrm{e}^{\frac{1}{2}J\frac{1}{a}J}\,, \tag{18}$$

where we computed the exactly solvable $Z_0(J)$. Calculating the interacting function $Z_\lambda(J)$ amounts to summing all orders of derivatives.

If we are only interested in the partition function $Z_\lambda = Z_\lambda(0)$, we have

$$\frac{Z_\lambda}{Z_0} = \frac{1}{Z_0}\int \mathrm{d}\phi\, \mathrm{e}^{-\frac{1}{2}a\phi^2}\mathrm{e}^{\lambda\phi^4} = \left\langle \mathrm{e}^{\lambda\phi^4}\right\rangle_0 = \sum_{n=0}^{\infty}\frac{\lambda^n}{n!}\langle\phi^{4n}\rangle_0\,.$$

Before turning to the field integral, let us consider the multi-dimensional generalization of the above toy problem. Defining vectors $\vec{\phi} = \{\phi_1, \dots, \phi_N\}$ (e.g., lattice sites) we can expand the partition function as

$$\begin{aligned}\frac{Z_\lambda}{Z_0} &= \frac{1}{Z_0}\int \left[\prod_i \mathrm{d}\phi_i\right] \mathrm{e}^{-\frac{1}{2}\sum_{ij}\phi_i A_{ij}\phi_j + \lambda\sum_i \phi_i^4} \\ &= \sum_{n=0}^{\infty}\frac{\lambda^n}{n!}\sum_{i_1}\cdots\sum_{i_n}\langle\phi_{i_1}\phi_{i_1}\phi_{i_1}\phi_{i_1}\cdots\phi_{i_n}\phi_{i_n}\phi_{i_n}\phi_{i_n}\rangle_0\,.\end{aligned} \tag{19}$$

where the ϕ^4 interaction terms can now appear at different sites i. The expectation values are calculated with a Gaussian action, and you have shown

in problem 5.1 that Wick's theorem allows us to decompose general expectation values into a sum over all possible pairings of variables ϕ. The proof was based on the generating function $Z_0(J)$ with a source term $\sum_i J_i\phi_i$ and

$$\langle\phi_{i_1}\phi_{i_2}\cdots\phi_{i_{4n}}\rangle_0 = \frac{\partial^{4n}}{\partial J_{i_1}\ldots\partial J_{i_{4n}}}\bigg|_{J=0} Z_0(J)\,.$$

Hence we can write $\langle\phi_{i_1}\phi_{i_2}\cdots\phi_{i_{4n}}\rangle_0$ as the sum over all possible ways (permutations P of the indices) of forming $2n$ pairs

$$\langle\phi_{i_1}\phi_{i_2}\cdots\phi_{i_{4n}}\rangle_0 = \sum_P A^{-1}_{i_1 i_{P1}} A^{-1}_{i_2 i_{P2}}\cdots A^{-1}_{i_{4n} i_{P2n}} \tag{20}$$

Here, A^{-1}_{ij} corresponds to the expectation value (Green function) $\langle\phi_i\phi_j\rangle_0 = G^0_{ij}$. The possible pairings may be depicted graphically. For a given n in equation (19), we have n vertices, each associated with four variables ϕ_i. The possible permutations in equation (20) correspond to the different ways of joining the $4n$ variables (lines). Each vertex gives a factor λ and a sum over the position i_p, while each line joining i_p and i_q gives a factor $G^0_{i_p i_q}$.

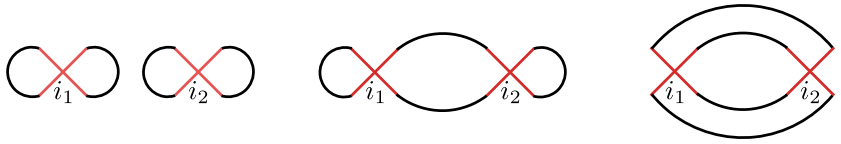


Figure 2: Second-order (λ^2) terms contributing to equation (19).

The three types of contractions of the second-order contribution $\langle\phi^4_{i_1}\phi^4_{i_2}\rangle_0$ are illustrated in figure 2. For A we contract only legs from the same vertex. Since there is a total of four pairs, we get

$$A = \frac{\lambda^2}{2!}\sum_{i_1}\sum_{i_2} G^0_{i_1 i_1} G^0_{i_1 i_1} G^0_{i_2 i_2} G^0_{i_2 i_2}\,.$$

For B, we have intra- and intervertex contractions, leading to

$$B = \frac{\lambda^2}{2!}\sum_{i_1}\sum_{i_2} G^0_{i_1 i_1} G^0_{i_1 i_2} G^0_{i_2 i_1} G^0_{i_2 i_2}\,.$$

Finally, for C we have only intervertex pairings,

$$C = \frac{\lambda^2}{2!} \sum_{i_1} \sum_{i_2} G^0_{i_1 i_2} G^0_{i_1 i_2} G^0_{i_2 i_1} G^0_{i_2 i_1} \, .$$

There are many ways (9, 72, 24) of selecting vertex legs to arrive at either A, B or C that all give the same contribution. Because we are considering the partition function, all diagrams correspond to so-called vacuum fluctuations without external lines. This changes if we consider Green functions between fixed external positions x and y. The first-order contributions to $\langle \phi(x)\phi(y) \rangle$ are shown in figure 3. $A = \lambda G^0_{xy} \sum_{i_1} G^0_{i_1 i_1} G^0_{i_1 i_1}$ corresponds to a disconnected diagram (the external fields do not couple to the vertex), while $B = \lambda \sum_{i_1} G^0_{x i_1} G^0_{i_1 i_1} G^0_{i_1 y}$ relates to a connected diagram.

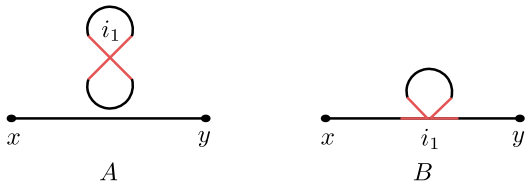


Figure 3: First order (λ) terms contributing to $\langle \phi(x)\phi(y) \rangle$.

The above ideas can be almost directly carried over to obtain a perturbation expansion for the coherent state path integral. For ϕ^4 theory (see page 19) we find, in almost perfect analogy with the continuum limit of equation (18),

$$\frac{Z_\lambda[J]}{Z_0[0]} = \mathrm{e}^{\frac{\lambda}{4!} \int \mathrm{d}^4 w (\delta/\delta J(w))^4} \mathrm{e}^{\frac{1}{2} \iint \mathrm{d}^4 x \, \mathrm{d}^4 y J(x) G(x-y) J(y)} \, .$$

Coming back to condensed-matter problems in the coherent state representation, we consider a Hamiltonian of the form $\hat{H} = \hat{H}_0 + \hat{V}$ with the one-particle part (kinetic energy; i, j encode lattices sites) $\hat{H}_0(a^\dagger, a) = \sum_{ij} t_{ij} a_i^\dagger a_j$ and the (normal-ordered) density-density interaction $\hat{V}(a^\dagger, a) = \sum_{ij} V_{ij} a_i^\dagger a_j^\dagger a_j a_i$. We write the functional integral representation of the partition function as

$$\begin{aligned} Z &= \int \mathcal{D}[\overline{\psi}, \psi] \mathrm{e}^{-\int_0^\beta \mathrm{d}\tau \left[\sum_{ij} \overline{\psi}_i(\tau) \left[(\partial_\tau - \mu)\delta_{ij} + t_{ij} \right] \psi_j(\tau) + \sum_{ij} V_{ij} \overline{\psi}_i(\tau) \overline{\psi}_j(\tau) \psi_j(\tau) \psi_i(\tau) \right]} \\ &= Z_0 \left\langle \mathrm{e}^{-\int_0^\beta \mathrm{d}\tau V(\overline{\psi}(\tau), \psi(\tau))} \right\rangle_0 \, . \end{aligned}$$

and expand Z/Z_0 as a series in powers of the interaction V,[38]

$$\begin{aligned}\frac{Z}{Z_0} &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta \mathrm{d}\tau_1 \cdots \int_0^\beta \mathrm{d}\tau_n \langle V(\overline{\psi}(\tau_1), \psi(\tau_1)) \cdots V(\overline{\psi}(\tau_n), \psi(\tau_n)) \rangle_0 \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta \mathrm{d}\tau_1 \cdots \int_0^\beta \mathrm{d}\tau_n \sum_{i_1 j_1} \cdots \sum_{i_n j_n} V_{i_1 j_1} \cdots V_{i_n j_n} \\ &\qquad \times \langle \overline{\psi}_{i_1}(\tau_1) \overline{\psi}_{j_1}(\tau_1) \psi_{j_1}(\tau_1) \psi_{i_1}(\tau_1) \cdots \overline{\psi}_{i_n}(\tau_n) \overline{\psi}_{j_n}(\tau_n) \psi_{j_n}(\tau_n) \psi_{i_n}(\tau_n) \rangle_0 \,,\end{aligned}$$

corresponding to a sum over all perturbation orders n and—for given n—all allowed vertex variables τ, i, j for each vertex. The expectation value is with respect to the noninteracting (Gaussian) problem defined by $\hat{H}_0$ and can be calculated with the help of Wick's Theorem. In the coherent state representation used here, the latter takes the form

$$\langle \psi_{i_1}(\tau_1) \cdots \psi_{i_n}(\tau_n) \overline{\psi}_{j_1}(\tau_1') \cdots \overline{\psi}_{j_n}(\tau_n') \rangle_0 = \sum_P \zeta^P G^0_{i_1 j_{P1}}(\tau_1, \tau'_{P1}) \cdots G^0_{i_n j_{Pn}}(\tau_n, \tau'_{Pn}) \,,$$

corresponding to all possible pairings (contractions) of one $\overline{\psi}$ and one ψ,

$$\langle \psi_i(\tau) \overline{\psi}_j(\tau') \rangle_0 = \psi_i \overbrace{(\tau) \overline{\psi}_j(\tau')} = G^0_{ij}(\tau, \tau') = \langle T[a_i(\tau) a_j^\dagger(\tau')] \rangle_0 \,.$$

The commutation properties of the fields also imply

$$\langle \overline{\psi}_j(\tau') \psi_i(\tau) \rangle_0 = \zeta \langle \psi_i(\tau) \overline{\psi}_j(\tau') \rangle_0 = \zeta G^0_{ij}(\tau, \tau') \,, \quad \overline{\psi}_j \overbrace{(\tau') \psi_i(\tau)} = \zeta \psi_i \overbrace{(\tau) \overline{\psi}_j(\tau')} \,.$$

The terms appearing in the perturbation expansion can again be interpreted diagrammatically. Here we consider the first-order term only. Wick's Theorem gives two contributions,

$$\begin{aligned} A + B &= -\int_0^\beta \mathrm{d}\tau \sum_{ij} V_{ij} \left[\overline{\psi}_i \overbrace{(\tau) \overline{\psi}_j \overbrace{(\tau) \psi_j \overbrace{(\tau) \psi_i(\tau)}}} + \overline{\psi}_i \overbrace{(\tau) \overline{\psi}_j \overbrace{(\tau) \psi_j \overbrace{(\tau) \psi_i(\tau)}}} \right] \\ &= -\int_0^\beta \mathrm{d}\tau \sum_{ij} V_{ij} \left[\overline{\psi}_i \overbrace{(\tau) \psi_i(\tau)} \overline{\psi}_j \overbrace{(\tau) \psi_j(\tau)} + \zeta \overline{\psi}_i \overbrace{(\tau) \psi_j(\tau)} \overline{\psi}_j \overbrace{(\tau) \psi_i(\tau)} \right] \end{aligned}$$

[38] This is the functional integral analogue of the Dyson expansion of the time-evolution operator in the interaction picture,

$$\frac{Z}{Z_0} = \langle \hat{U}_\mathrm{I}(\beta, 0) \rangle_0 = \langle T \mathrm{e}^{-\int_0^\beta V_\mathrm{I}(\tau)} \rangle_0 = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta \mathrm{d}\tau_1 \ldots \tau_n \langle T[\hat{V}_\mathrm{I}(\tau_1) \cdots \hat{V}_\mathrm{I}(\tau_n)] \rangle_0 \,.$$

In the second line, we have reordered the fields so that the contracted fields are next to each other, which gives the additional ζ in the second term. In the last step, we exchange the order of $\overline{\psi}$ and ψ (which gives a factor $\zeta^2 = 1$ and insert the Green functions:

$$A + B = -\int_0^\beta \mathrm{d}\tau \sum_{ij} V_{ij} \left[G^0_{ii}(\tau,\tau) G^0_{jj}(\tau,\tau) + \zeta G^0_{ji}(\tau,\tau) G^0_{ij}(\tau,\tau) \right] .$$

The interaction considered here has two incoming particles corresponding to ψ_j, ψ_i and two outgoing particles corresponding to $\overline{\psi}_i$, $\overline{\psi}_j$, and takes place at a single time τ. The vertex and the diagrams corresponding to the first-order terms A and B are shown in figure 4. A is the so-called Hartree term, corresponding to a density-density interaction $\langle \hat{n}_i \rangle \langle \hat{n}_j \rangle$,[39] while B is the Fock or exchange term, a purely quantum-mechanical contribution. The ideas

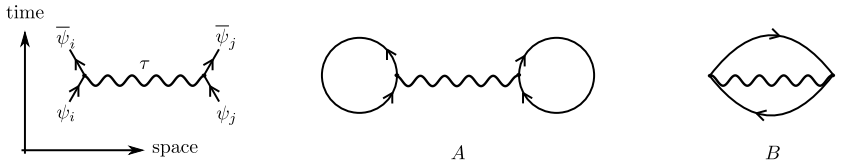


Figure 4: Vertex and first-order diagrams for the density-density interaction.

presented here are the starting point for a systematic expansion in terms of Feynman diagrams. Of particular importance for strongly correlated electrons is the identification and summation to infinite order of certain subclasses of important diagrams, and the possibility to sum *all* diagrams for a finite system using Monte Carlo simulations.

[39] Because time-ordering is not defined for equal times, the contraction $\overline{\psi}_j \overbrace{(\tau) \psi_i(\tau)}$ is defined such that ψ_i acts at $\tau - 0^+$. This implies that $\overline{\psi}_j \overbrace{(\tau) \psi_i(\tau)}(\tau,\tau) = \langle \hat{n}_i \rangle_0$.

Literature

The present lecture notes are largely based on material from the following sources, which are also good choices for further reading.

Quantum Field Theory for the Gifted Amateur
Lancaster, Blundell / Oxford University Press

Condensed Matter Field Theory
Altland, Simons / Cambridge University Press

Quantum Many-Particle Systems
Negele, Orland / Perseus Books

Quantum Field Theory in a Nutshell
Zee / Princeton University Press

Quantum Mechanics and Path Integrals
Feymman, Hibbs / Dover Books

Notes on (Semi-)Advanced Quantum Mechanics
Blau / `www.blau.itp.unibe.ch/Lecturenotes.html`

Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets
Kleinert / World Scientific

Notes from Sidney Coleman's Physics 253
Coleman / `http://arxiv.org/abs/1110.5013`

ABC of instantons
Vainshtein, Zakharov, Novikov, Shifman / Soviet Physics Uspekhi (1982)[40]

Viel-Teilchen-Theorie
Nolting / vieweg

Many-Body Quantum Theory in Condensed Matter Physics: An Introduction
Bruus, Flensberg / Oxford University Press

[40] Can be found on Google.