Lecture notes for PHYS503

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Contents

Chapter 1

Independent particles

In this section we discuss systems containing N identical, non-relativistic, non-interacting particles of spin S (S is an integer for bosons, a half-integer for fermions). In the *absence* of particle-particle interactions, the many-body problem always reduces to finding the solution of the one-particle problem. The many-body wave-functions are simply given by properly symmetrized/antisymmetrized products of one-particle bosonic/fermionic wave-functions. Here we discuss some techniques for finding the solutions to one-particle problems, such as Green's functions, path integrals, diagrammatics, etc. The idea is to get acquainted with these techniques and their meaning and applicability for this simpler case. We will then progress to the study of interacting many-body systems.

1.1 Quantum mechanics for a single particle - review of notation

The dynamics of the particle is described by some Hermitian Hamiltonian $\hat{H}$, acting on the one-particle Hilbert space $\mathcal{H}$. The Hilbert space is generally a product of Hilbert spaces associated with the translational and the spin degrees of freedom, $\mathcal{H} = \mathcal{H}_{tr} \otimes \mathcal{H}_{spin}$. However, sometimes we will "forget" about the spin degrees of freedom, and be concerned only with the location in space of the so-called "spinless" particle. In this case $\hat{H}$ contains no spin operators. Other times we will "forget" the translational degrees of freedom and concern ourselves only with the dynamics of localized spins – this works, for instance, in some insulators.

Examples of Hamiltonians:

$\hat{H} = \frac{\hat{\vec{p}}^2}{2m}$ $\quad \rightarrow$ free (possibly spinless) particle;

$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + V(\hat{\vec{r}}, t)$ $\quad \rightarrow$ particle in an some external field.

$\hat{H} = \frac{1}{2m}\left[\hat{\vec{p}} - q\vec{A}(\hat{\vec{r}}, t)\right]^2 + q\Phi(\hat{\vec{r}}, t) - g\mu_B \hat{\vec{S}} \cdot \vec{B}(\hat{\vec{r}}, t)$ $\quad \rightarrow$ spinful particle of charge q in an external classical electromagnetic field, $\vec{B} = \nabla \times \vec{A}, \vec{E} = -\nabla\Phi - \frac{\partial A}{\partial t}$.

$\hat{H} = \gamma \hat{\vec{S}} \cdot \vec{B}(t)$ $\quad \rightarrow$ localized particle in external magnetic field $\vec{B}(t)$. The list goes on and on.

Note: all quantities with a hat on are operators acting on the Hilbert space (sometimes trivially).

Sometimes we will work in an abstract Hilbert space, with abstract states denoted by $|\psi\rangle$. Sometimes, however, it is convenient to use particular representations, such as the $\vec{r}$-representation. In this case, we use the complete, orthonormal basis set for the Hilbert space:

$$|\vec{r}, S_z\rangle = |\vec{r}\rangle \otimes |S, S_z\rangle$$

where $\hat{\vec{r}}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle$ are eigenstates of the position operator, while $\hat{\vec{S}}^2 |S, S_z\rangle = \hbar^2 S(S+1)|S, S_z\rangle$,

$\hat{S}_z|S,S_z\rangle = \hbar S_z|S,S_z\rangle$ are eigenstates of the spin operators $\hat{\vec{S}}^2, \hat{S}_z$. It is convenient to introduce the simplified notation $x = (\vec{r}, S_z)$ such that $|x\rangle = |\vec{r}, S_z\rangle$. In this case, the orthonormation and the completeness relations are written as:

$$\langle x|x'\rangle = \langle \vec{r}|\vec{r}'\rangle\langle S,S_z|S,S_z'\rangle = \delta(\vec{r}-\vec{r}')\delta_{S_z,S_z'} = \delta_{x,x'} \tag{1.1}$$

and

$$\mathbf{1} = \sum_{S_z=-S}^{S}\int d\vec{r}|\vec{r},S_z\rangle\langle\vec{r},S_z| = \sum dx|x\rangle\langle x| \tag{1.2}$$

The last notation should hopefully remind us to sum over all discrete variables, and integrate over all continuous ones. In this basis, any state can be decomposed as:

$$|\psi\rangle = \sum dx\langle x|\psi\rangle|x\rangle = \sum_{S_z=-S}^{S}\int d\vec{r}\psi(\vec{r},S_z)|\vec{r},S_z\rangle$$

where $\psi(x) = \psi(\vec{r},S_z) = \langle\vec{r},S_z|\psi\rangle$, also known as the wavefunction, is the amplitude of probability that the particle in state $|\psi\rangle$ is at position $\vec{r}$ with spin S_z. This amplitude is generally a complex number. **Note:** if the particle has a finite spin $S > 0$, then $\langle\vec{r}|\psi\rangle$ is a spinor with $2S+1$ entries,

$$\langle\vec{r}|\psi\rangle = \psi(\vec{r}) = \begin{pmatrix} \psi(\vec{r},S) \\ \psi(\vec{r},S-1) \\ \dots \\ \psi(\vec{r},-S) \end{pmatrix}$$

Then, for instance, the probability to find the particle at $\vec{r}$ is $\psi^\dagger(\vec{r})\psi(\vec{r}) = \sum_{S_z}|\psi(\vec{r},S_z)|^2$, as expected. Clearly, if we know the wavefunctions $\psi(x)$, we know the state of the system. Any equation for $|\psi\rangle$ can be turned into an equation for $\psi(x)$ by simply acting on it with $\langle x|$: $|\psi_1\rangle = |\psi_2\rangle \to \psi_1(x) = \psi_2(x)$. However, we also have to deal with expression of the form $\langle x|\hat{A}|\psi\rangle$, where $\hat{A}$ is some abstract operator. In fact, the only operators that appear in the Hamiltonian are (combinations of):

$$\langle x|\hat{\vec{r}}|\psi\rangle = \vec{r}\psi(\vec{r},S_z)$$

$$\langle x|\hat{\vec{p}}|\psi\rangle = -i\hbar\nabla\psi(\vec{r},S_z)$$

$$\langle x|\hat{S}_z|\psi\rangle = \hbar S_z\psi(\vec{r},S_z); \quad \langle x|\hat{S_\pm}|\psi\rangle = \hbar\sqrt{(S\mp S_z)(S\pm S_z+1)}\psi(\vec{r},S_z\pm 1)$$

where $\hat{S_\pm} = \hat{S}_x \pm i\hat{S}_y$. In general, $\langle x|\hat{A}|\psi\rangle = \sum dx'\langle x|\hat{A}|x'\rangle\psi(x')$. As long as we can compute the matrix elements of the operator in the basis of interest, we have its representation in that basis.

Again, note that if we project on $\langle\vec{r}|$ only, these are equations for spinors. In this case, the last equation changes to a matrix equation

$$\langle\vec{r}|\hat{S}_z|\psi\rangle = \tilde{S}_z\psi(\vec{r}) = \begin{pmatrix} \hbar S & 0 & \dots & 0 \\ 0 & \hbar(S-1) & \dots & 0 \\ \dots & \dots & \dots & 0 \\ 0 & 0 & 0 & -\hbar S \end{pmatrix}\begin{pmatrix} \psi(\vec{r},S) \\ \psi(\vec{r},S-1) \\ \dots \\ \psi(\vec{r},-S) \end{pmatrix}$$

i.e. each spin-component gets multiplied by its particular spin projection. One can also find the matrix representations for the operators $\hat{S}_x, \hat{S}_y$ (**exercise** - do it!).

Example: consider a spin-$\frac{1}{2}$ particle in an external magnetic field, described by the abstract Hamiltonian

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} - \gamma \hat{\vec{S}} \cdot \vec{B}(t)$$

In the $\vec{r}$-representation, the Schrödinger equation $i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$ can be written in a compact form, as a spinor equation:

$$i\hbar \frac{d\psi(\vec{r})}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 - \gamma \tilde{\vec{S}} \cdot \vec{B}(t) \right] \psi(\vec{r})$$

where

$$\psi(\vec{r}) = \begin{pmatrix} \psi(\vec{r}, \uparrow) \\ \psi(\vec{r}, \downarrow) \end{pmatrix}$$

and the spin-$\frac{1}{2}$ matrices are $\tilde{S}_i = \frac{\hbar}{2}\sigma_i$, where the matrices σ are called the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

You should convince yourselves that the equations for the wavefunctions $\psi(\vec{r}, S_z)$ that we obtain by projecting the abstract equation onto $\langle \vec{r}, S_z|$ are equivalent to this spinor equation.

All this may seem rather trivial and somewhat of a waste of time. However, the reason I explicitly showed this here is because we will proceed very similarly when we will use different representations. The other representation you may be familiar with is the $\vec{p}$-representation, where one works in $\vec{k}$-space instead of the real space, by projecting onto the $|\vec{k}, S_z\rangle$ basis. However, we will also use coherent basis states instead of the $|\vec{r}\rangle$ basis and/or the $|S, S_z\rangle$ basis, etc. No matter what basis of the Hilbert space we choose, we can derive the representations of the abstract equations in a similar way. While formulations in different representations are all equivalent, some may be more convenient for particular types of calculations, than others.

1.2 The time-evolution operator

The evolution of the system is governed by the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle \tag{1.3}$$

subject to some initial condition $|\psi(t = t_0)\rangle = |\psi_0\rangle$. This equation allows us to find the evolution of the state describing the system if we know the initial state, provided that we can integrate this differential equation. The problem with direct integration is that every time we change the initial state, we have to redo the calculation. One way to avoid this is to define a **time-evolution operator** $\hat{U}(t, t_0)$ such that:

$$|\psi(t)\rangle = \hat{U}(t, t_0)|\psi(t_0)\rangle \tag{1.4}$$

If we know this operator, we can find the state of the system for any possible initial state. $\hat{U}$ must be a unitary operator $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = 1$, in order to insure the conservation of probability $\langle\psi(t)|\psi(t)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle$.

From Schrödinger's equation (1.3) and definition (1.4), the time-evolution operator is given by:

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0); \qquad \hat{U}(t_0,t_0) = 1. \tag{1.5}$$

The formal solution is:

$$\hat{U}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} d\tau \hat{H}(\tau)\hat{U}(\tau,t_0) \tag{1.6}$$

and can be solved by iterations to give:

$$\hat{U}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} d\tau \hat{H}(\tau) + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} d\tau_1 \hat{H}(\tau_1)\int_{t_0}^{\tau_1} d\tau_2 \hat{H}(\tau_2) + ...$$

The higher-order terms in this infinite sum can be forced to have all integrals on the $[t_0, t]$ interval. Since in general $\hat{H}(\tau_1)\hat{H}(\tau_2) \neq \hat{H}(\tau_2)\hat{H}(\tau_1)$, one has to be careful of the order in which the operators corresponding to different times are listed.

We define the time-ordering operator:

$$\mathbf{T}\left\{\hat{H}(\tau_1)\hat{H}(\tau_2)\dots\hat{H}(\tau_n)\right\} = \hat{H}(\tau_{P_1})\hat{H}(\tau_{P_2})\dots\hat{H}(\tau_{P_n}) \tag{1.7}$$

where $(P_1, \dots, P_n)$ is the permutation of the indexes $(1, \dots, n)$ for which $\tau_{P_1} \geq \tau_{P_2} \geq \dots \geq \tau_{P_n}$. In other words, it simply orders the operators it acts upon in decreasing order of time. **Note:** when acting on operators other than Hamiltonians, the time-ordering operator has a more general definition. We will introduce it when necessary.

You should now verify that:

$$\hat{U}(t,t_0) = \sum_{n\geq 0}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} d\tau_1 \int_{t_0}^{t} d\tau_2 \dots \int_{t_0}^{t} d\tau_n \mathbf{T}\left\{\hat{H}(\tau_1)\hat{H}(\tau_2)\dots\hat{H}(\tau_n)\right\} = \mathbf{T}e^{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau \hat{H}(\tau)} \tag{1.8}$$

Here the second equality defines a simplified notation, so that we do not have to write this sum explicitly every time we refer to the time-evolution operator.

Exercise: show that if the Hamiltonian is time-independent, then

$$\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} \tag{1.9}$$

This is the situation we will generally be interested in.

1.3 Green's functions or propagators

The definition of the **propagator** or **Green's function** in the abstract formulation is simply:

$$\hat{\mathcal{G}}(t_f,t_i) = \Theta(t_f - t_i)\hat{U}(t_f,t_i) = \Theta(t_f - t_i)\mathbf{T}e^{-\frac{i}{\hbar}\int_{t_i}^{t_f} d\tau \hat{H}(\tau)} \tag{1.10}$$

and shows that the propagator characterizes the evolution of the particle between the initial time t_i and a *later* final time t_f (the Heaviside function $\Theta(x) = 1$ if $x > 0$ and vanishes otherwise). Strictly speaking, this is the *retarded* Green's function. One could also define an advanced Green's function for $t_f < t_i$. However, for the single-particle case we can extract all the information needed from the retarded propagator. In the following I will not use the label retarded.

Properties of the propagator:

$$\hat{\mathcal{G}}(t_f,t_i) = \hat{\mathcal{G}}(t_f,t_{n-1})\hat{\mathcal{G}}(t_{n-1},t_{n-2})\cdots\hat{\mathcal{G}}(t_2,t_i) \tag{1.11}$$

for any sequence of intermediary times $t_i = t_1 < t_2 < \ldots < t_{n-1} < t_n = t_f$. In other words, the evolution of the system from the initial to the final time is the product of evolutions from the initial to the first intermediary time, followed by the evolution to the second next intermediary time, etc. The equation of evolution of the propagator can be obtained, using Eq. (1.5):

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}(t)\right)\hat{\mathcal{G}}(t,t_0) = i\hbar\delta(t-t_0) \tag{1.12}$$

The presence of the δ term is why this is called a Green's function – Green's functions have such equations of motion. Sometimes, it is convenient to use a slightly different definition of the Green's function, according to the equation of evolution:

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}(t)\right)\hat{G}(t,t_0) = \delta(t-t_0) \tag{1.13}$$

Clearly,

$$\hat{G}(t,t_0) = -\frac{i}{\hbar}\hat{\mathcal{G}}(t,t_0) = -\frac{i}{\hbar}\Theta(t_f-t_i)\hat{U}(t_f,t_i) = -\frac{i}{\hbar}\Theta(t_f-t_i)\mathbf{T}e^{-\frac{i}{\hbar}\int_{t_i}^{t_f}d\tau\hat{H}(\tau)} \tag{1.14}$$

If the Hamiltonian is time-independent, then $\hat{G}(t,t_0) = \hat{G}(t-t_0)$ where [see Eq. (1.9)]:

$$\hat{G}(t) = -\frac{i}{\hbar}\hat{\mathcal{G}}(t) = -\frac{i}{\hbar}\Theta(t)e^{-\frac{i}{\hbar}\hat{H}t} \tag{1.15}$$

A time-independent Hamiltonian has a complete basis state $\hat{H}|n\rangle = E_n|n\rangle$, where $\sum|n\rangle\langle n| = 1$. It follows that:

$$\hat{G}(t) = -\frac{i}{\hbar}\Theta(t)\sum_n e^{-\frac{i}{\hbar}E_n t}|n\rangle\langle n| \tag{1.16}$$

Whenever the Hamiltonian is time-independent, the total energy of the system is conserved. As a result, it is more convenient to work in the frequency-domain than in the time-domain. We begin with a Fourier transform of Eq. (1.16). The convention we use for Fourier transform in the time-domain is always:

$$f(t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}f(\omega); \quad f(\omega) = \int_{-\infty}^{\infty}dt e^{i\omega t}f(t) \tag{1.17}$$

For an energy $E = \hbar\omega$, we find:

$$\hat{G}(E) = -\frac{i}{\hbar}\sum_n|n\rangle\langle n|\int_{-\infty}^{\infty}dt\Theta(t)e^{\frac{i}{\hbar}(E-E_n)t}$$

The proper way to perform such integrals is to use the following representation of the Heaviside function (see Appendix 1):

$$\Theta(t) = \lim_{\eta\to 0} i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{\omega+i\eta}$$

The time integral is now trivial, and we find:

$$\hat{G}(E) = -\frac{i}{\hbar}\hat{\mathcal{G}}(E) = \sum_n\frac{|n\rangle\langle n|}{E-E_n+i\eta} = \frac{1}{E-\hat{H}+i\eta} \tag{1.18}$$

This provides an alternative definition of the Green's function in the frequency-domain (used as the starting point in many textbooks):

$$\left(E-\hat{H}+i\eta\right)\hat{G}(E) = \hat{G}(E)\left(E-\hat{H}+i\eta\right) = 1 \tag{1.19}$$

Note: this definition is less general than Eq. (1.10), since it applies only to time-independent Hamiltonians. A similar equation can be found for the advanced Green's function, the only difference is that $i\eta \to -i\eta$ (or $\Theta(t_f - t_i) \to \Theta(t_i - t_f)$, in the time-domain).

Let us now discuss the $\vec{r}$-representations of these equations, since we rarely work directly in the abstract space. Remember the notation $x = (\vec{r}, S_z)$. We define:

$$\mathcal{G}(x_f, t_f; x_i, t_i) = \langle x_f | \hat{\mathcal{G}}(t_f, t_i) | x_i \rangle \tag{1.20}$$

What is the meaning of this quantity? Assume that at $t = t_i$, the particle is in state $|x_i\rangle$, i.e. at point $\vec{r}_i$ with spin $S_{z,i}$. At time t, then, the state of the particle will be [Eq. (1.4)]:

$$|\psi(t)\rangle = \hat{U}(t, t_i)|x_i\rangle$$

and the amplitude of probability to find the system in state $|x_f\rangle$ at $t = t_f$ is simply $\langle x_f|\psi(t_f)\rangle = \langle x_f|\hat{U}(t_f, t_i)|x_i\rangle = \langle x_f|\hat{\mathcal{G}}(t_f, t_i)|x_i\rangle$ if $t_f > t_i$.

Thus, the propagator $\mathcal{G}(x_f, t_f; x_i, t_i)$ is the *amplitude of probability that the particle which was in state x_i (at position $\vec{r}_i$ with spin $S_{z,i}$) at the initial moment t_i, will be found in state x_f (at position $\vec{r}_f$ with spin $S_{z,f}$) at a later time t_f*. It is important to remember this physical meaning of the propagator – it will make diagrammatic much more easy to understand and intuitive.

If we know the propagator, we can easily find the evolution of wave-functions:

$$\psi(x_f, t_t) = \langle x_f|\psi(t_f)\rangle = \sum dx_i \mathcal{G}(x_f, t_f; x_i, t_i)\psi(x_i, t_i)$$

i.e. the sum over all the ways for the particle to evolve from any possible initial position into the final desired one. The analog of Eq. (1.11) also has a straightforward interpretation. If we use a single intermediary time and insert a resolution of identity $\sum dx|x\rangle\langle x| = 1$, we find:

$$\mathcal{G}(x_f, t_f; x_i, t_i) = \sum dx \mathcal{G}(x_f, t_f; x, t)\mathcal{G}(x, t; x_i, t_i) \tag{1.21}$$

for any $t_i < t < t_f$. The total amplitude of probability to evolve from (x_i, t_i) to (x_f, t_f) is the product of amplitudes of probability to evolve from (x_i, t_i) to (x, t), at some intermediary time t, and then from (x, t) to (x_f, t_f). Since x could be anywhere, in order to find the total amplitude we need to sum all the possibilities, i.e. over all allowed x values. This can be generalized to n intermediary points; it is knows as the Trotter formula and is the starting point for path-integral techniques.

For time-independent Hamiltonians, we find from Eq. (1.18) that:

$$G(x_f, x_i; E) = \langle x_f|\hat{G}(E)|x_i\rangle = \sum_n \frac{u_n(x_f)u_n^*(x_i)}{E - E_n + i\eta} \tag{1.22}$$

where $u_n(x) = \langle x|n\rangle$ are the eigenstates of the system. We see that in the frequency-domain, *the poles of the Green's function correspond to the eigenenergies of the Hamiltonian, while the residues are related to the eigenfunctions.*

Another useful identity for time-independent systems is the **Feynman-Kac formula** which links statistical mechanics and the quantum evolution of the system. The partition function is given by:

$$\mathcal{Z} = Tre^{-\beta\hat{H}} = \sum_n e^{-\beta E_n} = \sum dx \sum_n e^{-\beta E_n}\langle x|n\rangle\langle n|x\rangle = \sum dx \mathcal{G}(x, -i\hbar\beta; x, 0)$$

where we used the normalization condition $\langle n|n\rangle = \sum dx\langle n|x\rangle\langle x|n\rangle = 1$, and Eq. (1.15).

We can use this to calculate the expectation value of any operator:

$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_n e^{-\beta E_n} \langle n|\hat{O}|n\rangle = \frac{1}{Z} \int_{-\infty}^{\infty} dE e^{-\beta E} \mathrm{Tr}(\hat{A}(E)\hat{O})$$

where

$$\hat{A}(E) = \sum_n \delta(E - E_n)|n\rangle\langle n| = -\frac{1}{\pi}\mathrm{Im}\hat{G}(E)$$

This function $A(E)$ is actually important enough to have its own name: the spectral function. It has the property that:

$$\int_{-\infty}^{\infty} dE \hat{A}(E) = \hat{1}$$

Usually one encounters it in some specific representation. For instance:

$$\langle x|\hat{A}(E)|x\rangle = \sum_n \delta(E - E_n)|u_n(x)|^2 = -\frac{1}{\pi}\mathrm{Im}G(x, x; E)$$

is the so-called local density of states (LDOS). It tells us the probability to find electrons with energy E located at x. If we integrate over all x, we find the total density of states. Etc.

To summarize: if we know $\mathcal{G}(x_f, t_f; x_i, t_i)$ or $G(x_f, x_i; E)$, we know how the system evolves in time, and therefore we can compute any expectation value and solve any problem of interest. The question, then, is how to calculate these Green's functions?

1.4 Finding the propagators for time-independent Hamiltonians

There are several convenient methods to compute the propagators, depending on the specific $\hat{H}$.

1.4.1 Direct integration

If the Hamiltonian is simple enough, one can compute it directly from the definitions of the previous section. *Simple enough* generally means that we know its complete basis of eigenstates, $H\psi_n(\vec{r}, S_z) = E_n\psi_n(\vec{r}, S_z)$. In this case, all is needed is to be able to perform the sum/integral in Eq. (1.22).

Example: Green's function for free spinless particle in 1D, $G_0(x_2, x_1; E)$. Attention, here x is a position along the 1D line, and there is no spin quantum number. The eigenstates and eigenfunctions are simple planewaves, $u_k(x) = e^{ikx}/\sqrt{2\pi}$. Then, Eq. (1.22) reads:

$$G_0(x_f, x_i; E) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{-ik(x_f - x_i)}}{E - \frac{\hbar^2 k^2}{2m} + i\eta} = -i\frac{m}{\hbar^2 k_0} e^{ik_0|x_f - x_i|} \tag{1.23}$$

where $E = \frac{\hbar^2 k_0^2}{2m}$. Note that the sign of $i\eta$ is essential in determining the position of the poles. Another example (assignment) is a tight-binding Hamiltonian, $\hat{H}_0 = -t\sum_n (|n\rangle\langle n+1| + h.c.)$.

1.4.2 Solving Dyson's equation exactly

More typical is the case where $\hat{H} = \hat{H}_0 + \hat{V}$, where $\hat{H}_0$ is a simple enough Hamiltonian for which we can compute explicitly $\hat{G}_0 = 1/\left(E - \hat{H}_0 + i\eta\right)$. By definition:

$$\left(E - \hat{H} + i\eta\right)\hat{G}(E) = 1 \rightarrow \left(E - \hat{H}_0 + i\eta\right)\hat{G}(E) = 1 + \hat{V}\hat{G}(E)$$

Multiplying from the left with $\hat{G}_0(E)$, we obtain **Dyson's equation**:

$$\hat{G}(E) = \hat{G}_0(E) + \hat{G}_0(E)\hat{V}\hat{G}(E) = \hat{G}_0(E) + \hat{G}(E)\hat{V}\hat{G}_0(E) \tag{1.24}$$

Note: these operators generally do not commute, so the second identity is not trivial. You should be able to obtain it starting from $\hat{G}(E)\left(E - \hat{H} + i\eta\right) = 1$. Dyson's formula is a self-consistent equation for the Green's function. In the x-representation, assuming a potential $\hat{V}(\vec{r}, \vec{S})$, Dyson's equation is:

$$G(x_2, x_1; E) = G_0(x_2, x_1; E) + \sum dx G_0(x_2, x; E)V(x)G(x, x_1; E) \tag{1.25}$$

Sometimes this self-consistent equation can be solved explicitly. Let's consider several examples:

Example 1: free spinless particle in 1D, subject to a scattering potential $V(x) = v\delta(x)$. In other words, depending on whether v is positive or negative, the particle is strongly repulsed or attracted to the origin (for instance, by some impurity placed there). Again, in 1D for a spinless particle, x is simply the position of the particle. Dyson's equations becomes:

$$G(x_2, x_1; E) = G_0(x_2, x_1; E) + \int_{-\infty}^{\infty} dx G_0(x_2, x; E)V(x)G(x, x_1; E)$$

$$= G_0(x_2, x_1; E) + vG_0(x_2, 0; E)G(0, x_1; E) \xrightarrow{x_2=0} G(0, x_1; E) = \frac{G_0(0, x_1; E)}{1 - vG_0(0, 0; E)} \rightarrow$$

$$G(x_2, x_1; E) = G_0(x_2, x_1; E) + v\frac{G_0(x_2, 0; E)G_0(0, x_1; E)}{1 - vG_0(0, 0; E)}$$

Substituting the expression for G_0 from Eq. (1.23), we have the full solution. Remember that poles of $G(E)$ correspond to eigenenergies. This means that we might have a new eigenstate if $1 - vG_0(0, 0; E) = 0$. Clearly, if $E \geq 0$ (spectrum for free particle) this equation has no solution. However, for $E < 0$ and $v < 0$ (i.e., only for attractive potential), we find a new solution $k_0 = i\sqrt{2m|E|/\hbar^2} = -ivm/\hbar^2 \rightarrow |E| = |v|^2 m/(2\hbar^2)$. We can also infer that this is a bound solution, localized near $x = 0$, from the residue of G at this particular energy. Basically, since k_0 is imaginary, from Eq. (1.23) it follows that at this energy, the nominator decreases exponentially away from 0.

If you want some practice, you could try to generalize this analysis to 2 and 3 dimensions, and see whether there is always a bound state for a δ-function attractive potential. You can also investigate how to generalize this approach in 1D, for a sum of several δ-function potentials. The problem can still be solved exactly (at least numerically). Of course, for such simple systems we could also directly solve Schödinger's equation to find the bound states, with the same results.

Example 2: Let us assume we know the Green's function of a spinless particle on an infinite tight-binding chain, $G_0(n, m; E)$, corresponding to $\hat{H}_0 = -t\sum_n (|n\rangle\langle n+1| + h.c.)$. What is the Green's function for a semi-infinite chain?

First, we need to express the Hamiltonian of the semi-infinite chain as $\hat{H} = \hat{H}_0 + \hat{V}$. What is $\hat{V}$? Let's assume that the chain is cut between sites 0 and 1. For sites on the same side of the cut, $n, m \leq 0$ or $n, m \geq 1$, we must have $\langle n|\hat{H}|m\rangle = \langle n|\hat{H}_0|m\rangle \rightarrow \langle n|\hat{V}|m\rangle = 0$, i.e. there is no change because of the cut. However, if $n \leq 0$ and $m \geq 1$ or viceversa, since the chain is cut there must be no connections between such sites, and therefore here $\langle n|\hat{H}|m\rangle = 0 \rightarrow \langle n|\hat{V}|m\rangle = -\langle n|\ H_0|m\rangle = t\delta_{n,0}\delta_{m,1} + t\delta_{n,1}\delta_{m,0}$. Knowledge of all the matrix elements of $\hat{V}$ gives us $\hat{V} = +t\,(|0\rangle\langle 1| + |1\rangle\langle 0|)$. This should be no surprise, since adding this $\hat{V}$ to $\hat{H}_0$ precisely cancels any hopping between sites 0 and 1, "cutting" the chain into two semi-infinite halves. For a general potential, Dyson's equation is:

$$G(n_2, n_1; E) = G_0(n_2, n_1; E) + \sum_{m_1, m_2} G_0(n_2, m_2; E)\langle m_2|\hat{V}|m_1\rangle G(m_1, n_1; E)$$

Remember that $G(n_2, n_1; E)$ is related to the amplitude of probability to move from site n_1 to site n_2. If the chain is cut, this must be zero if n_1 is on one side of the cut, and n_2 is on the other side (of course, this can be shown explicitly from the calculation - try it). Let's say then that we are interested in the right-hand semi-infinite chain, with $n_2, n_1 \geq 1$ (I will use the subscript R). The potential has non-zero matrix elements only if $m_1 = 0, m_2 = 1$ or viceversa. Since $n_1 \geq 1$ and the chain is cut, $G_R(0, n_1; E) = 0$ and thus only $m_1 = 1$, $m_2 = 0$ contributes:

$$G_R(n_2, n_1; E) = G_0(n_2, n_1; E) + tG_0(n_2, 0; E)G_R(1, n_1; E) \rightarrow G_R(1, n_1; E) = \frac{G_0(1, n_1; E)}{1 - tG_0(1, 0; E)} \rightarrow$$

$$G_R(n_2, n_1; E) = G_0(n_2, n_1; E) + t\frac{G_0(n_2, 0; E)G_0(1, n_1; E)}{1 - tG_0(1, 0; E)}$$

You can similarly find the Green's function for the left-side semi-infinite chain. Again, we see that G_R has new poles (meaning new eigenstates) at energies E for which $1 - tG_0(1, 0; E)$. If such solutions exist, they would correspond to *surface states*, i.e. to wavefunctions bound near the cut, which decay exponentially away from the cut. The 1D tight-binding Hamiltonian is too simple and does not support such surface states, but more general Hamiltonians usually do (for instance, consider the case where every second site of the chain has an onsite potential U_0, such that $\hat{H}_0 = -t\sum_n (|n\rangle\langle n+1| + h.c.) + U_0 \sum_n |2n\rangle\langle 2n|$. Is there a surface state?).

This general approach can now be used to find the Green's function for a finite chain, by making a second cut; or we could consider "re-joining" two semi-infinite chains, one with hopping t_L and one with hopping t_R together and finding that Green's function; or we could add some on-site impurities, etc. Murray's project from last year did a nice analysis of how impurity states emerge from the continuum when you add a large enough impurity potential.

In conclusion, there are a number of cases where the Green's function can be obtained directly from Dyson's equation. This is generally the case when V has a finite number of non-zero matrix elements, making the Dyson's equation into a finite system of coupled equations that can be solved exactly. However, this is rather the exception, not the rule.

1.4.3 Solving Dyson's equation approximatively

Using iterations, we can find the solution of Dyson's equation as the infinite series:

$$\hat{G}(E) = \hat{G}_0(E) + \hat{G}_0(E)\hat{V}\hat{G}_0(E) + \hat{G}_0(E)\hat{V}\hat{G}_0(E)\hat{V}\hat{G}_0(E) + \ldots \tag{1.26}$$

This suggests an approximative solution, which works only if $\hat{V}$ is a perturbation. In this case, higher order terms in this infinite expansion become smaller and smaller and can be neglected. In particular, if we stop after the first term:

$$\hat{G}(E) \approx \hat{G}_0(E) + \hat{G}_0(E)\hat{V}\hat{G}_0(E) \tag{1.27}$$

we obtain the so-called **Born approximation**. Notice that if we make such a truncation, no matter how many terms we keep in the expansion, we will never find "bound states" of the type described before, because there are no extra poles in the denominators. To understand this, consider a somewhat similar expansion $f(t) = 1 + t + t^2 + ...$ If we sum all (infinite number of terms), $f(t) = 1/(1-t)$ has a pole at $t = 1$. If we truncate the summation after n terms, we have $f_n(t) = 1 + \ldots + t^{n-1} = (1 - t^n)/(1 - t) \rightarrow f_n(1) = n =$ finite, no matter how large n is. It is important to realize that perturbational expansions like in Eq. (1.26) are only meaningful for energies E where $t = |\hat{V}\hat{G}_0(E)| < 1$, otherwise the series is not convergent.

Let us introduce some rather trivial diagrammatic notation – it is not necessary in this simple case, but it will help illustrate how this works in more complicated cases.

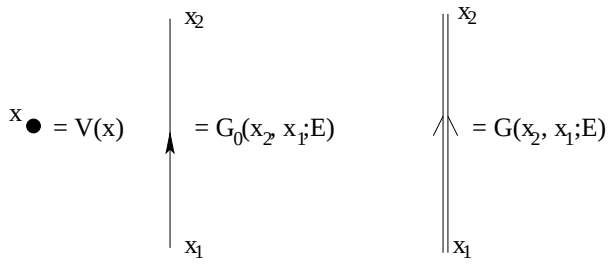

Figure 1.1: Diagrams for $V(x)$, $G_0(x_2, x_1; E)$ and $G(x_2, x_1; E)$.

Rule: If a "position" x is not specified by the initial or final points, we must sum over all possible x values. With these conventions, Dyson's equation (1.25), (1.26) are "depicted" in Fig. (1.2).

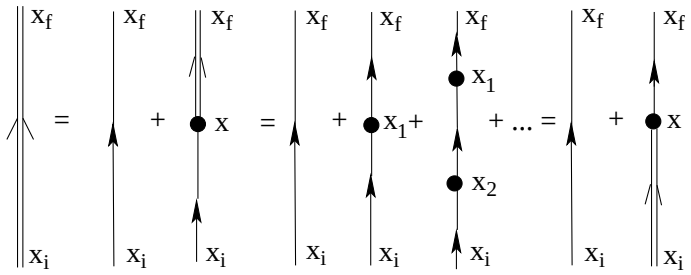

Figure 1.2: Dyson's equation in compact form and as an infinite series.

Notice that we can demonstrate the identity $GVG_0 = G_0VG$ trivially using diagrams.

Physical meaning: remember that $G(x_f, x_i)$ is related to the amplitude of probability for the particle to evolve from x_i to x_f. $G_0(x_f, x_i)$ is related to the amplitude of probability that the particle evolves from x_i to x_f without scattering (no interactions, $V = 0$). Dyson's formula is then simply the quantum mechanics rule that the total amplitude of probability for a process is the sum of amplitudes of probabilities of all possible ways in which the process can occur: the particle can go from x_i to x_f without any scattering (amplitude $G_0(x_f, x_i; E)$); or it can go without scattering up to some point x_1, where it scatters once, after which it goes to x_f without further scattering. Since x_1 can be anywhere, we must sum over all possibilities, so the contribution of the single-scattering processes is $\sum dx_1 G_0(x_f, x_1; E)V(x_1)G_0(x_1, x_i; E)$. But it is possible that the particle will scatter twice, or three times, or any number of times. The corresponding diagrams simply give us the amplitude of probability for such processes. (If the scattering is weak, for example because the density of impurities is very low the probability to scatter twice or more times is very small and can be neglected; keeping only the contribution of the single-scattering processes is, as I said, the so-called Born approximation. In the context of diagrammatics, there is something somewhat different that is also called a Born approximation - it consists of keeping only the first diagram in the self-energy expansion. More about this later).

Besides being a nice shorthand notation for complicated and/or long mathematical expressions, diagrams are very useful for approximations. When unable to sum all the diagrams, we will keep the ones which we believe are physically most relevant, and using diagrammatics will allow us to figure more easily how to sum them. This will begin to make more sense as we study more examples.

1.5 Green's functions in disordered systems

In the previous section, we discussed the Green's function in presence of some disorder potential, $V(\vec{r})$. Clearly, G depends on the particular V: if we change the positions of the impurities somewhat, V changes and so does G. When computing various quantities, we would like to find the *disorder averaged* values, i.e. the result we would obtain if we measured the same quantity for many different samples, and then averaged. This is the case, for instance, for macroscopic ("infinite size") systems. We can think of them as being made of finite-size subsystems which have all the possible disorder realizations, so the total result is the average over all possible disorders. This is called "self-averaging". (Of course, there are no infinite size systems. The requirement is that they are much larger than some particular lengthscales, having to do with the mean free path, with decoherence lengths, etc.)

Let us discuss how to compute the *disorder averaged* Green's functions, which we will denote by:

$$\bar{G}(\vec{r}_2, \vec{r}_1; E) = \langle G(\vec{r}_2, \vec{r}_1; E) \rangle_{dis} \tag{1.28}$$

Note: if V does not depend on spin operators, which we assume to be the case here for simplicity, then there is zero probability for the electron to have its spin flipped as it moves through the system. As a result, $G(\vec{r}_2\sigma_2, \vec{r}_1\sigma_1; E) = \delta_{\sigma_1,\sigma_2} G(\vec{r}_2, \vec{r}_1; E)$, and we can "forget" the spin degree of freedom.

We need some assumptions about the disorder. We assume Gaussian random disorder, defined as:

$$\langle V(\vec{r}) \rangle_{dis} = 0; \quad \langle V(\vec{r_1}) V(\vec{r_2}) \rangle_{dis} = W(\vec{r_1} - \vec{r_2}) \tag{1.29}$$

and for averages involving more potentials we use simple factorization. Let $V_1 \equiv V(\vec{r_1})$, etc. Then $\langle V_1 V_2 V_3 \rangle_{dis} = \langle V_1 V_2 \rangle \langle V_3 \rangle + ... = 0$, no matter how we factorize. Clearly, odd numbers of potentials always average to zero (roughly speaking, the potential at a point is positive in half the cases and negative in the other half, so averaging over an odd product should produce zero. Of course, if the potential is purely repulsive, you would expect the average to be positive. However, one can always redefine the energy scale and shift it such that $\langle V \rangle = 0$). On the other hand, $\langle V_1 V_2 V_3 V_4 \rangle_{dis} = \langle V_1 V_2 \rangle \langle V_3 V_4 \rangle + \langle V_1 V_3 \rangle \langle V_2 V_4 \rangle + \langle V_1 V_4 \rangle \langle V_2 V_3 \rangle = W(\vec{r_1} - \vec{r_2}) W(\vec{r_3} - \vec{r_4}) + W(\vec{r_1} - \vec{r_3}) W(\vec{r_2} - \vec{r_4}) + W(\vec{r_1} - \vec{r_4}) W(\vec{r_2} - \vec{r_3})$. Similar factorizations in products of two-point correlations apply to all higher, even orders. (One can demonstrate these identities starting from a gaussian distribution of probabilities for the disorder potentials. I will probably give you an assignment problem with an example of a disorder potential that behaves like this. For the moment, suffice it to say that such potentials exist, and they are called Gaussian random disorder).

Let us now perform the disorder average of Dyson's equation. All the terms which have an odd power of V average to zero. We have (see Eq. (1.26)):

$$\bar{G}(\vec{r}_f, \vec{r}_i; E) = G_0(\vec{r}_f, \vec{r}_i; E) + \langle \int d\vec{r}_1 \int d\vec{r}_2 G_0(\vec{r}_f, \vec{r}_1; E) V(\vec{r}_1) G_0(\vec{r}_1, \vec{r}_2; E) V(\vec{r}_2) G_0(\vec{r}_2, \vec{r}_i; E) \rangle_{dis} + ...$$

$$= G_0(\vec{r}_f - \vec{r}_i; E) + \int d\vec{r}_1 \int d\vec{r}_2 G_0(\vec{r}_f - \vec{r}_2; E) G_0(\vec{r}_2 - \vec{r}_1; E) W(\vec{r}_2 - \vec{r}_1) G_0(\vec{r}_1 - \vec{r}_i; E) + ... \tag{1.30}$$

Here it is already more convenient to work directly with diagrams. We introduce a new element – a dashed line – to stand for $W(\vec{r} - \vec{r}')$, where $\vec{r}, \vec{r}'$ are the end points of the dashed line. I will also use a thick double line for the averaged Green's function. Dyson's equation is shown in Fig. 1.3. The first two terms are the ones explicitly written in Eq. (1.30) and I added the next order terms, coming from averages of the 4^{th} power terms in V. Here you can already see that diagrams are much more convenient to draw than it is to write all the integrals by hand.

A very important fact to notice, is that $\bar{G}(\vec{r}_f, \vec{r}_i; E) = \bar{G}(\vec{r}_f - \vec{r}_i; E)$. Performing the disorder average has restored the invariance to translations, since there is now no difference between any

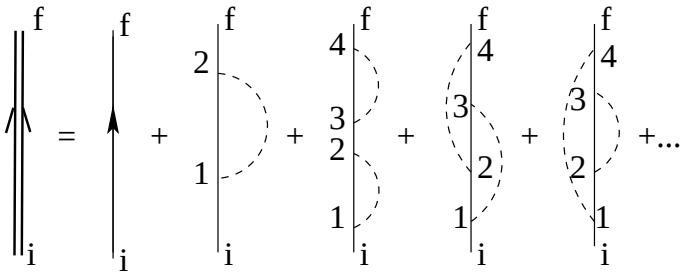

Figure 1.3: Dyson's equation for the disorder averaged Green's function.

points in space. (For each individual disorder realizations, different points have different values of the potential and each $G(\vec{r}_f, \vec{r}_i; E)$ depends explicitly on both points, not only on the distance between them. After averaging over all disorder realizations, there is no more difference between different areas of the sample, and the Green's function depends only on the distance between points, not on where are the points located, or how are they oriented in space with respect to one another). As always, in translationally-invariant cases it is convenient to Fourier transform and work in $\vec{k}$-space, because the momentum is conserved. Let us verify this:

$$\bar{G}(\vec{k}', \vec{k}; E) = \langle \vec{k}' | \bar{\hat{G}}(E) | \vec{k} \rangle = \int d\vec{r} \int d\vec{r}' \langle \vec{k}' | \vec{r}' \rangle \bar{G}(\vec{r}' - \vec{r}; E) \langle \vec{r} | \vec{k} \rangle = \delta_{\vec{k},\vec{k}'} \bar{G}(\vec{k}; E)$$

where

$$\bar{G}(\vec{k}; E) = \int d\vec{\rho} e^{-i\vec{k}\cdot\vec{\rho}} \bar{G}(\vec{\rho}; E)$$

In other words, the evolution of the electron is such that its initial and final momenta are equal (conserved), $\vec{k} = \vec{k}'$. Using the direct Fourier transforms:

$$G_0(\vec{\rho}; E) = \frac{1}{V} \sum_k e^{i\vec{k}\cdot\vec{\rho}} \bar{G}_0(\vec{k}; E); \quad W(\vec{\rho}) = \frac{1}{V} \sum_k e^{i\vec{k}\cdot\vec{\rho}} W(\vec{k})$$

Dyson's equation in $\vec{k}$-space representation becomes:

$$\bar{G}(\vec{k}; E) = G_0(\vec{k}; E) + \frac{1}{V} \sum_{\vec{q}} G_0(\vec{k}; E) \bar{G}_0(\vec{k} - \vec{q}; E) W(\vec{q}) G_0(\vec{k}; E) + ... \tag{1.31}$$

The meaning of these processes is straightforward. The first term is just the contribution of the electron of momentum $\vec{k}$ propagating through the system without scattering. The second term corresponds to the electron starting with its initial momentum; it then scatters elastically and looses some of its momentum, and propagates with $\vec{k} - \vec{q}$ for awhile. The "missing" momentum has been transferred to the impurities, but is recuperated after the second scattering (initial and final momenta are the same). Since any momentum $\vec{q}$ could be exchanged, we must sum over all possible values (if you prefer integrals, replace $(1/V) \sum_{\vec{k}} \to \int d\vec{k}/(2\pi)^3$). Again, things become more transparent in diagrammatic notation. The diagrams in $\vec{k}$-space are similar to those in real space, the only difference being that now each line carries a momentum, instead of being determined by initial and final points – see Fig. 1.4.

Dyson's equation looks similar to Fig. 1.3, except that now lines carry momenta, which are such that the total is conserved at each vertex. The only rule is to sum over all momenta which are not determined by the initial $\vec{k}$. Notice that except for the first term, all other terms begin and end with

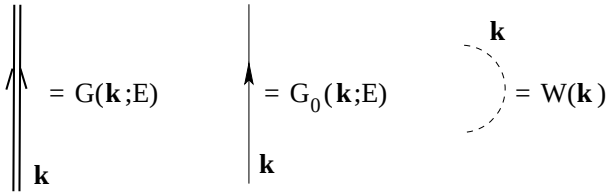

Figure 1.4: Meaning of $\vec{k}$-space diagrams.

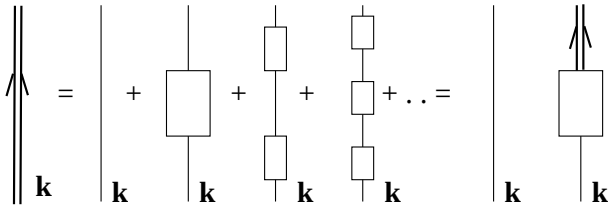

Figure 1.5: Dyson's equation in $\vec{k}$-space, resummed.

$G_0(\vec{k};E)$ and have "something" in the middle. In fact, we can resum diagrams as shown in Fig. 1.5:

The new diagram introduced is called the **proper self-energy** $\Sigma(\vec{k};E)$, and is given by an infinite sum of diagrams beginning and ending with a vertex (see Fig. 1.6), and which cannot be separated into similar diagrams by deletion of a single propagator line. Note that the *improper* diagram correspoding to the 3rd term in Fig. 1.3 is missing from Σ, although it is included in the total $\bar{G}$.

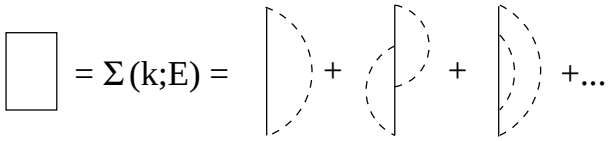

Figure 1.6: The proper self-energy, $\Sigma(\vec{k};E)$.

The second equality in Fig. 1.5 gives a implicit equation for $\bar{G}$, namely:

$$\bar{G}(\vec{k};E) = G_0(\vec{k};E) + G_0(\vec{k};E)\Sigma(\vec{k};E)\bar{G}(\vec{k};E) \rightarrow \bar{G}(\vec{k};E) = \frac{1}{G_0^{-1}(\vec{k};E) - \Sigma(\vec{k};E)} \tag{1.32}$$

For free particles:

$$G_0(\vec{k};E) = \langle\vec{k}|\frac{1}{E - \hat{H}_0 + i\eta}|\vec{k}\rangle = \frac{1}{E - \epsilon(\vec{k}) + i\eta} \tag{1.33}$$

where $\epsilon(\vec{k}) = \hbar^2k^2/(2m)$ is the free-particle dispersion. It follows that the exact solution for the disorder-averaged Green's function is:

$$\bar{G}(\vec{k};E) = \frac{1}{E - \epsilon(\vec{k}) - \Sigma(\vec{k};E) + i\eta} \tag{1.34}$$

This looks quite similar to the expression of G_0, except that the free-particle energy $\epsilon(\vec{k})$ is supplemented by Σ (this is why Σ is called self-energy – it characterizes a change in the eigenstate energies due to interactions). The new eigenstates are obtained from the poles of $\bar{G}$:

$$E - \epsilon(\vec{k}) - \Sigma(\vec{k};E) = 0$$

Notes: a) if Σ is independent of E, the new eigenenergies are $E = \epsilon(\vec{k}) + \Sigma(\vec{k})$, i.e. the overall effect of the interactions is to simply change the dispersion. You are already familiar with such a case: when dealing with electrons in a crystal, we account for the interaction with the periodic lattice by changing the bare electron mass into an effective mass, i.e. a change of the dispersion. b) it is possible that the self-energy is a complex number, in which case the eigenenergies acquire an imaginary part. This signals that these eigenstates have a *finite lifetime*. More about this later.

The problem of evaluating $\bar{G}$ has now been replaced with the problem of evaluating Σ. As usual, we have to make some approximation. The simplest would be to keep only the first term in Fig. 6, in which case

$$\Sigma(k,\omega) \approx \Sigma^{(1)}(\vec{k},E) = \int \frac{d\vec{q}}{(2\pi)^3} W(\vec{q}) G_0(\vec{k}-\vec{q};E)$$

Note that this approximation (also called the Born approximation) still implies summing an infinite number of diagrams in $\bar{G}$, shown in Fig. 1.7. This is very different from truncating directly in Dyson's equation, and summing only a finite number of diagrams. In fact, approximations where one keeps only a finite number of diagrams are generally useless (meaningless) exactly for energies we're most interested in, and we'll never encounter any other such examples.

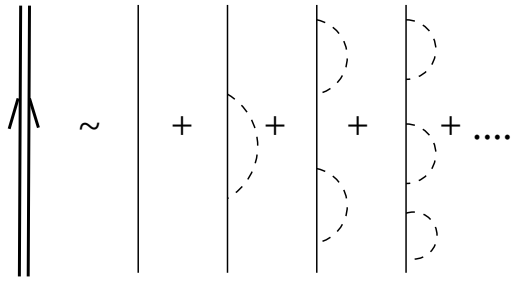

Figure 1.7: Diagrams kept in $\bar{G}$ if we truncate Σ to only the first term – the Born approximation.

The usual approximation one makes is the **self-consistent Born approximation** – SCBA. It consists of the self-consistent set of equations depicted in Fig. 1.8:

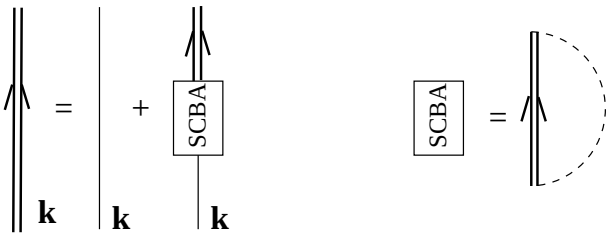

Figure 1.8: The self-consistent Born approximation.

$$\bar{G}_{SCBA}(\vec{k};E) = G_0(\vec{k};E) + G_0(\vec{k};E)\Sigma_{SCBA}(\vec{k};E)\bar{G}_{SCBA}(\vec{k};E) \tag{1.35}$$

where

$$\Sigma_{SCBA}(\vec{k};E) = \int \frac{d\vec{q}}{(2\pi)^3} W(\vec{q}) \bar{G}_{SCBA}(\vec{k}-\vec{q};E) \tag{1.36}$$

This approximation implies that one keeps in $\bar{G}_{SCBA}$ all possible **non-crossed** diagrams, such as the ones shown in Fig. 1.9. This is a *semi-classical approximation*. It can be shown to be valid (in

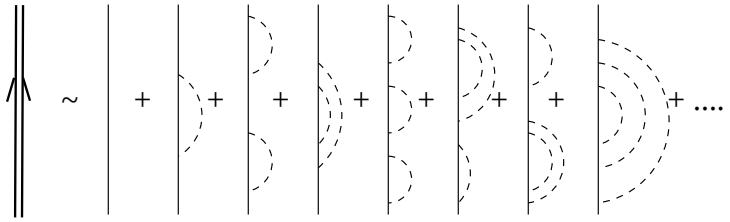

Figure 1.9: Non-crossed diagrams kept in $\bar{G}$ in the self-consistent Born approximation.

the sense that the neglected diagrams are much smaller than the diagrams there were kept) when $k_F l \gg 1$, where l is the mean-free path (average distance between successive scatterings) and k_F is the Fermi wavevector. This condition is satisfied in clean metals, which have many electrons (large k_F) and few impurities (large l). For instance, if used to evaluate the conductivity, this approximation reproduces the Drude result. Last year, Rodrigo did this calculation for his project, so you can read more about it there.

We can understand intuitively why this is a semi-classical approximation: all crossed diagrams, such as the 4th one in Fig.1.3, describe interference effects with one scattering process beginning before the previous one is finished. If we want to neglect interference effects (semi-classical calculation), we should ignore these diagrams. On the other hand, to understand the main quantum corrections to a semi-classical approximation, one needs to consider contributions from the "maximally-crossed diagrams". This is an interesting topic related to weak localization due to enhanced backscattering, and would make a good end-of-term project. However, we have to move on.

The goal of this section was to illustrate the power of diagrammatics. We can easily visualize and perform formal summation of infinite series (such as in Fig. 1.5). In turn, this allows us to make better approximations for the propagators, which include an infinite subset of the possible processes.

1.6 Finding the propagators for time-dependent Hamiltonians

In this section we will derive Dyson's equation for the case where $\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$ – the particle is interacting with some time-dependent external field. This derivation is similar in spirit to the one for many-body systems, but is easier to follow. In general, we cannot work in the frequency domain, so we have to work with the full $\hat{\mathcal{G}}(t_2, t_1) = \Theta(t_2 - t_1)\hat{U}(t_2, t_1)$. We already know from Eq. (1.8) that $\hat{U}(t_2, t_1) = \mathbf{T} \exp\left(-\frac{i}{\hbar}\int_{t_1}^{t_2} d\tau[\hat{H}_0 + \hat{V}(\tau)]\right)$, but usually we cannot evaluate this expression. Expansion and truncation are messy, since various terms contain mixed powers of $\hat{H}_0$ and $\hat{V}$.

We assume that we know the complete basis of $\hat{H}_0$, $\hat{H}_0|n\rangle = E_n|n\rangle$. We would like to factorize from $\hat{U}$ the entire evolution due to $\hat{H}_0$ exactly, and then see how we can deal with contributions from $\hat{V}$. To do this, we switch from the Schrödinger to the Interaction picture (index I), with the unitary transformation:

$$|\Psi_I(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}|\Psi(t)\rangle \tag{1.37}$$

From the Schrödinger equation $i\hbar d/dt|\Psi\rangle = \hat{H}|\Psi\rangle$, it follows immediately that

$$i\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle = \hat{V}_I(t)|\Psi_I(t)\rangle \tag{1.38}$$

where

$$\hat{V}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{V}(t)e^{-\frac{i}{\hbar}\hat{H}_0 t} \tag{1.39}$$

Note: even if $\hat{V}$ is time independent, $\hat{V}_I(t)$ has explicit time dependence.

We now define the time-evolution operator in the interaction picture as $|\Psi_I(t)\rangle = \hat{U}_I(t,t_0)|\Psi_I(t_0)\rangle$. Using the same arguments as before, we find that

$$\hat{U}_I(t,t_0) = \mathbf{T}e^{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau \hat{V}_I(\tau)} \tag{1.40}$$

Notice that unlike the expression for U, the series expansion for U_I contains only powers of V. We can now move back to the Schrödinger picture:

$$|\Psi(t)\rangle = \exp(-\frac{i}{\hbar}H_0 t)|\Psi_I(t)\rangle = \exp(-\frac{i}{\hbar}H_0 t)\hat{U}_I(t,t_0)|\Psi_I(t_0)\rangle = \hat{U}(t,t_0)|\Psi(t_0)\rangle \rightarrow$$

$$\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_I(t,t_0)e^{\frac{i}{\hbar}\hat{H}_0 t_0} \tag{1.41}$$

and thus

$$\hat{\mathcal{G}}(t,t_0) = \Theta(t-t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t}\left[\mathbf{T}e^{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau \hat{V}_I(\tau)}\right]e^{\frac{i}{\hbar}\hat{H}_0 t_0} \tag{1.42}$$

Let us now write explicitly the infinite series denoted by $[\mathbf{T}\ldots]$, and also use Eq. (1.39) to express everything in terms of $\hat{V}(t)$. We have:

$$\hat{\mathcal{G}}(t,t_0) = \Theta(t-t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t}\left[1 + \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t} d\tau e^{\frac{i}{\hbar}\hat{H}_0\tau}\hat{V}(\tau)e^{-\frac{i}{\hbar}\hat{H}_0\tau}\right.$$

$$\left. + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} d\tau_1 e^{\frac{i}{\hbar}\hat{H}_0\tau_1}\hat{V}(\tau_1)e^{-\frac{i}{\hbar}\hat{H}_0\tau_1}\int_{t_0}^{\tau_1} d\tau_2 e^{\frac{i}{\hbar}\hat{H}_0\tau_2}\hat{V}(\tau_2)e^{-\frac{i}{\hbar}\hat{H}_0\tau_2} + \ldots\right]e^{\frac{i}{\hbar}\hat{H}_0 t_0}$$

But $\hat{\mathcal{G}}_0(t,t_0) = \Theta(t-t_0)\exp[-\frac{i}{\hbar}\hat{H}_0(t-t_0)]$, i.e. all the exponentials are just "unperturbed" propagators, in the absence of $\hat{V}$. We thus obtain **Dyson's equation**:

$$\hat{\mathcal{G}}(t,t_0) = \hat{\mathcal{G}}_0(t,t_0) + \int_{t_0}^{t} d\tau \hat{\mathcal{G}}_0(t,\tau)\left[-\frac{i}{\hbar}\hat{V}(\tau)\right]\hat{\mathcal{G}}_0(\tau,t_0)$$

$$+ \int_{t_0}^{t} d\tau_1 \int_{t_0}^{\tau_1} d\tau_2 \hat{\mathcal{G}}_0(t,\tau_1)\left[-\frac{i}{\hbar}\hat{V}(\tau_1)\right]\hat{\mathcal{G}}_0(\tau_1,\tau_2)\left[-\frac{i}{\hbar}\hat{V}(\tau_2)\right]\hat{\mathcal{G}}_0(\tau_2,t_0) + \ldots \rightarrow$$

$$\hat{\mathcal{G}}(t,t_0) = \hat{\mathcal{G}}_0(t,t_0) + \int_{t_0}^{t} d\tau \hat{\mathcal{G}}_0(t,\tau)\left[-\frac{i}{\hbar}\hat{V}(\tau)\right]\hat{\mathcal{G}}(\tau,t_0) \tag{1.43}$$

(If you are wondering about the $-i/\hbar$ factors, remember that that was exactly the difference between G and $\mathcal{G}$. You should verify that if $\hat{V}$ is time-independent, Eqs. (1.43) and (1.24) are equivalent. In x-representation, this becomes simply:

$$\mathcal{G}(x_f,t_f;x_i,t_i) = \mathcal{G}_0(x_f,t_f;x_i,t_i) + \int_{t_0}^{t} d\tau \sum dx \mathcal{G}_0(x_f,t_f;x,\tau)\left[-\frac{i}{\hbar}V(x,\tau)\right]\mathcal{G}(x,\tau;x_i,t_i)$$

We can again introduce simple diagrams for these terms. They look similar to those of Fig. 1.1, except that now we specify both positions and times x_i,t_i, x_f,t_f and that $\bullet$ stands for $(-i/\hbar)V(x,\tau)$. The meaning is again very transparent. For instance, $\rightarrow \bullet \rightarrow$ describes a particle propagating freely from the initial point (x_i,t_i) to some intermediary point (x,τ) where it scatters, after which it propagates freely to the end. If we want the total amplitude of probability for such processes, we must sum (integrate) over all the possible times $t_i < \tau < t_f$ and all allowed spatial/spin x values.

All the ideas introduced in the previous section, such as defining a self-energy etc, can be duplicated here as well.

Conclusion: except in very special cases, we generally *cannot* sum the infinite series of diagrams to find the exact $\mathcal{G}$ or G propagators. We can, however, find an approximate solution by expanding in powers of V and adding only some of the resulting diagrams. Such approximations are justified if and only the neglected terms are "small", and therefore are perturbational schemes. If there are no "small" parameters in the problem, we need different approaches, such as path integral formulations. We will discuss these next.

1.7 Path integrals for spinless particles

For simplicity of notation, let us assume 1D motion along the Ox axis, no external EM fields and no intrinsic time dependence of the Hamiltonian. Generalization to account for higher dimensionality, etc, is straightforward. The Hamiltonian, in the x-representation, is

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) = T + V \tag{1.44}$$

We would like to evaluate the propagator

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

in a "non-perturbative" manner, i.e. treating the kinetic and the potential energies on equal footing.

We use the identity $\exp(A) = [\exp(\frac{A}{N})]^N$. Then, $\exp(-\lambda H) = \exp(-\frac{\lambda}{N}H)\cdots\exp(-\frac{\lambda}{N}H)$, where the product has N terms and we use the shorthand notation

$$\lambda = \frac{i}{\hbar}(t_f - t_i) \tag{1.45}$$

Next, we factorize each term in the product:

$$e^{-\frac{\lambda}{N}H} = e^{-\frac{\lambda}{N}(T+V)} = e^{-\frac{\lambda}{N}T}e^{-\frac{\lambda}{N}V} + \mathcal{O}\left(\frac{\lambda^2}{N^2}\right)$$

Proof: let $f(x) = \exp(xV)\exp[-x(T+V)]\exp(xT) \rightarrow f(0) = 1;\ f'(0) = 0$ and therefore $f(x) \approx 1 + \mathcal{O}(x^2)$. For $x = \lambda/N \ll 1$, we obtain the above equation. Combining all this, we find:

$$e^{-\lambda H} = \left[e^{-\frac{\lambda}{N}T}e^{-\frac{\lambda}{N}V} + \mathcal{O}\left(\frac{\lambda^2}{N^2}\right)\right]^N \overset{N\to\infty}{\longrightarrow} \left[e^{-\frac{\lambda}{N}T}e^{-\frac{\lambda}{N}V}\right]^N + \mathcal{O}\left(\frac{\lambda}{N}\right)$$

This is not a rigorous derivation, but the result is correct. This is the **Trotter product formula**:

$$\mathcal{G}(x_f, t_f; x_i, t_i) = \Theta(t_f - t_i)\lim_{N\to\infty}\langle x_f | \left[e^{-\frac{\lambda}{N}T}e^{-\frac{\lambda}{N}V}\right]^N | x_i\rangle \tag{1.46}$$

Let us introduce $N-1$ intermediary points in the (x_i, x_f) interval; we use the notation $x_i \equiv x_0 < x_1 < x_2 < \ldots < x_N \equiv x_f$. For each intermediary point we use a resolution of identity $\int_{-\infty}^{\infty} dx_i |x_i\rangle\langle x_i| = 1$ and insert it between terms in the Trotter formula. We assume $t_f > t_i$, and we do not write explicitly the Heaviside function (but it is there). We have:

$$\mathcal{G}(x_f, t_f; x_i, t_i) = \lim_{N\to\infty}\prod_{i=1}^{N-1}\int_{-\infty}^{\infty} dx_i \langle x_N | e^{-\frac{\lambda}{N}T}e^{-\frac{\lambda}{N}V} | x_{N-1}\rangle\langle x_{N-1}| e^{-\frac{\lambda}{N}T}e^{-\frac{\lambda}{N}V}|x_{N-2}\rangle\cdots\langle x_1|e^{-\frac{\lambda}{N}T}e^{-\frac{\lambda}{N}V}|x_0\rangle$$

Note: this is really just a generalization of Eq. (1.21) – the evolution of the particle from initial to final state is a product of its evolution through intermediary points (which could be anywhere) at intermediary times $t_n = t_i + n(t_f - t_i)/N$, $n = 0, ..., N$.

We now need to evaluate the matrix elements. This is a straightforward task:

$$\langle x_{j+1}|e^{-\frac{\lambda}{N}T}e^{-\frac{\lambda}{N}V}|x_j\rangle = e^{-\frac{\lambda}{N}V(x_j)}\int_{-\infty}^{\infty}dk\langle x_{j+1}|k\rangle\langle k|e^{-\frac{\lambda}{N}T}|x_j\rangle = e^{-\frac{\lambda}{N}V(x_j)}\int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{-\frac{\lambda}{N}\frac{\hbar^2k^2}{2m}+ik(x_{j+1}-x_j)}$$

The main formula one needs to know in dealing with path integrals is the **Gaussian integral**:

$$\int_{-\infty}^{\infty}dxe^{-ax^2+bx} = \sqrt{\frac{\pi}{a}}e^{\frac{b^2}{4a}} \tag{1.47}$$

which gives us:

$$\langle x_{j+1}|e^{-\frac{\lambda}{N}T}e^{-\frac{\lambda}{N}V}|x_j\rangle = \sqrt{\frac{mN}{2\pi\hbar^2\lambda}}e^{-\frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\hbar^2\lambda/N}-\frac{\lambda}{N}V(x_j)}$$

Let us define the time step

$$\epsilon = \frac{t_f - t_i}{N} \to \frac{\hbar\lambda}{N} = i\epsilon$$

Putting this all together, we get:

$$\mathcal{G}(x_f,t_f;x_i,t_i) = \lim_{N\to\infty}\int_{-\infty}^{\infty}dx_1\cdots\int_{-\infty}^{\infty}dx_{N-1}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N}{2}}e^{\frac{i}{\hbar}\epsilon\sum_{j=0}^{N-1}\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2-V(x_j)\right]} \tag{1.48}$$

This might seem very complicated, but in fact it has a very nice interpretation. Let us first understand the meaning of the product of integrals. What we did is to divide the time interval in steps of ϵ, after each time step the particle is at a new point x_j. The set of points (x_0, t_0), (x_1, t_1), ..., (x_N, t_N) describes a possible trajectory between the initial and the final points, which are fixed. Since the intermediary positions can vary anywhere in space, integrating over all of them means adding contributions from all the possible paths that start at (x_i, t_i) and end at (x_f, t_f) – see Fig. 1.10. But what are we summing? In the $N \to \infty$ limit, and because $\delta t = \epsilon$, we have

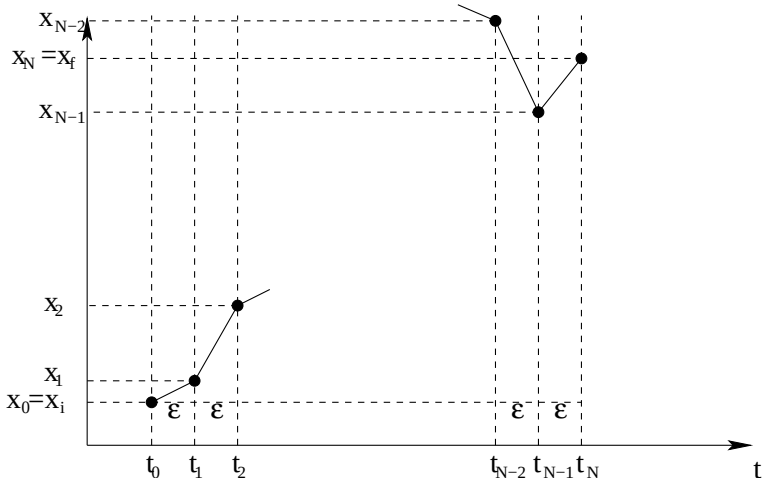

Figure 1.10: Path (trajectory) between initial and final points.

$$\sum_{j=0}^{N-1}\epsilon\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2 - V(x_j)\right] \overset{N\to\infty}{\longrightarrow} \int_{t_i}^{t_f}d\tau\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 - V(x)\right] = \int_{t_i}^{t_f}d\tau\mathcal{L} = S[x]$$

This is just the classical action S for this path $x(\tau)$, $\mathcal{L} = T - V$ being the classical Lagrangian. So the conclusion is that

$$\mathcal{G}(x_f, t_f; x_i, t_i) = \sum_{\substack{\text{all paths} \\ \substack{x(t_i)=x_i \\ x(t_f)=x_f}}} e^{\frac{i}{\hbar}S[x]} = \int \mathcal{D}[x(\tau)] e^{\frac{i}{\hbar}S[x]} \tag{1.49}$$

The second equality just introduces the typical notation for a path integral. The mathematical meaning of this notation is the limit of Eq. (1.48). The physical meaning is that the amplitude of probability for a particle to move from the initial to the final point is the sum of amplitudes of probabilities for it to evolve on any possible path (sum over histories); for each path, the amplitude of probability is given by the exponential of the action along that path. Thinking in such terms makes paradoxical quantum mechanical effects such as the two-slit experiment easier to understand.

The classical limit $\hbar \to 0$ can be easily recovered. For two neighboring paths $x_2(t) = x_1(t) + \delta x(t)$, we have $S_2 - S_1 = \delta S = \int_{t_i}^{t_f} d\tau \delta x(\tau) \frac{\delta S}{\delta \tau}$. For a large (classical) object $\delta S \gg \hbar$ and therefore the phase difference varies fast and randomly for neighboring trajectories, canceling out their contributions. Only neighboring paths for which $\delta S = 0$ can interfere constructively and give a finite contribution. These are the paths close to $x_{cl}(t)$ for which $\delta S/\delta x = 0$, i.e. the classical trajectory itself.

Before moving on, let us remember the Feynman-Kac formula, which allows us to perform finite-temperature calculations by using the imaginary time $\Delta t \to -i\beta\hbar$, where $\beta = 1/(k_B T)$. If we define the step $\bar{\epsilon} = \beta\hbar/N$ and repeat the calculation, we find:

$$\langle x_f | e^{-\beta H} | x_i \rangle = \lim_{N\to\infty} \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_{N-1} \left(\frac{m}{2\pi\hbar\bar{\epsilon}}\right)^{\frac{N}{2}} e^{\frac{i}{\hbar}\int_0^{\beta\hbar}(-id\tau)\left[\frac{m}{2}\left(\frac{dx}{-id\tau}\right)^2 - V(x)\right]} \to$$

$$\langle x_f | e^{-\beta H} | x_i \rangle = \int \mathcal{D}[x(\tau)] e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau H} \tag{1.50}$$

In this case, the Hamiltonian of the system appears in the exponent instead of the Lagrangian.

Notes: (1) you should now be able to figure out the generalizations for higher dimensionality etc. As long as you know the classical Lagrangian/Hamiltonian, things are quite simple. (2) You might wonder what would happen if instead of the factorization $\exp(-\lambda T/N)\exp(-\lambda V/N)$ we would have used $\exp(-\lambda V/N)\exp(-\lambda T/N)$ or some other combination. In this case, in the exponent of Eq. (1.48) we would have $V(x_{j+1})$, but we could also have the symmetric form $1/2[V(x_j) + V(x_{j+1})]$. For a simple Hamiltonian like in Eq. (1.44), all these forms give the same result. One has to be careful and more rigorous if the Hamiltonian contains terms like xp_x whose order is important in quantum mechanics, but makes no difference in a classical Lagrangian. (3) Most importantly, notice that in this approach T and V are treated on equal footing. This is *not* a perturbational approach in V, like the diagrammatic expansions. We should therefore expect non-perturbational contributions.

The physical interpretation of Eq. (1.49) is very satisfying, but we still have to figure out how to compute that quantity. In a small number of cases, one can use brute-force integration of Eq. (1.48). We will do this for a free particle in 1D, and for variety we will do it at finite T. In this case (see formula before Eq. (1.50)), we have to calculate:

$$\langle x_f | e^{-\beta H} | x_i \rangle = \lim_{N\to\infty} \int_{-\infty}^{\infty} dx_1 \ldots \int_{-\infty}^{\infty} dx_{N-1} \left(\frac{m}{2\pi\hbar\bar{\epsilon}}\right)^{\frac{N}{2}} e^{-\frac{\bar{\epsilon}}{\hbar}\sum_{j=0}^{N-1}\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\bar{\epsilon}}\right)^2}$$

where $\bar{\epsilon} = \hbar\beta/N$. We collect all terms containing x_1 and perform the first gaussian integral:

$$\int_{-\infty}^{\infty} dx_1 \sqrt{\frac{m}{2\pi\hbar\bar{\epsilon}}} e^{-\frac{m}{2\hbar\bar{\epsilon}}\left[(x_1-x_0)^2 + (x_2-x_1)^2\right]} = \ldots = \frac{1}{\sqrt{2}} e^{-\frac{m}{2\hbar 2\bar{\epsilon}}(x_2-x_0)^2}$$

Collecting terms containing x_2, we then find:

$$\frac{1}{\sqrt{2}}\int_{-\infty}^{\infty} dx_2 \sqrt{\frac{m}{2\pi\hbar\bar{\epsilon}}} e^{-\frac{m}{2\hbar 2\bar{\epsilon}}(x_2-x_0)^2-\frac{m}{2\hbar\bar{\epsilon}}(x_3-x_2)^2} = \ldots = \frac{1}{\sqrt{3}} e^{-\frac{m}{2\hbar 3\bar{\epsilon}}(x_3-x_0)^2}$$

By induction, after the integral over x_{N-1} we have:

$$\langle x_f|e^{-\beta H}|x_i\rangle = \lim_{N\to\infty} \frac{1}{\sqrt{N}} \sqrt{\frac{m}{2\pi\hbar\bar{\epsilon}}} e^{-\frac{m}{2\hbar N\bar{\epsilon}}(x_N-x_0)^2} = \sqrt{\frac{m}{2\pi\hbar^2\beta}} e^{-\frac{m}{2\hbar^2\beta}(x_f-x_i)^2}$$

since $N\bar{\epsilon} = \hbar\beta$. Using analytical continuation to $\Delta t = -i\beta\hbar$ we find:

$$\mathcal{G}_0(x_f,t_f;x_i,t_i) = \Theta(t_f-t_i)\sqrt{\frac{m}{2\pi i\hbar\Delta t}} e^{i\frac{m}{2\hbar\Delta t}(x_f-x_i)^2} \tag{1.51}$$

This is a very useful result which is needed to derive the propagators in more complicated cases [and agrees with Eq. (1.23)]. Note that for any potential that is up to quadratic in x, we can use the gaussian integrals to perform these integrals and therefore we could find the solution in this way. Again, cases where we can do it are rather the exception than the rule. In fact, in these cases we can always find the propagator by some simpler method than doing the path integral. However, for complicated Hamiltonians, doing the path integrals is the method of choice to obtain rather easily non-perturbational results.

1.7.1 General method to compute the path integral

We would like to calculate:

$$\mathcal{G}(x_f,t_f;x_i,t_i) = \Theta(t_f-t_i)\int \mathcal{D}[x(\tau)] e^{\frac{i}{\hbar}S[x]}$$

where $x(t_i) = x_i, x(t_f) = x_f$ and for each path, the action is:

$$S[x] = \int_{t_i}^{t_f} d\tau \left[\frac{m}{2}\dot{x}^2 - V(x)\right]$$

Step 1: Find the classical solution $x_{cl}(t)$ from the Euler-Lagrange equation:

$$\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{x}}\right) = \frac{\partial\mathcal{L}}{\partial x}$$

We will use as an example the simple harmonic oscillator (SHO), for which $V(x) = kx^2/2$. The solution for the equation of motion $m\ddot{x} = -kx$ satisfying the initial/final constraints is

$$x_{cl}(t) = \frac{x_f - x_i\cos(\omega\Delta t)}{\sin(\omega\Delta t)} \cdot \sin[\omega(t-t_i)] + x_i\cos[\omega(t-t_i)]$$

where $\omega = \sqrt{k/m}$ and $\Delta t = t_f - t_i$.

Step 2: Any trajectory $x(t)$ satisfying the constraints is of general form $x(t) = x_{cl}(t) + y(t)$, where $y(t_i) = y(t_f) = 0$. We rewrite the path integral in terms of y:

$$\mathcal{G}(x_f,t_f;x_i,t_i) = \Theta(t_f-t_i)\int_{y(t_i)=0}^{y(t_f)=0} \mathcal{D}[y(\tau)] e^{\frac{i}{\hbar}S[x_{cl}+y]}$$

We now expand the action functional:

$$S[x_{cl}+y] = S[x_{cl}] + \int_{t_i}^{t_f} d\tau \left.\frac{\delta S}{\delta x}\right|_{x=x_{xl}} \cdot y(\tau) + \frac{1}{2}\int_{t_i}^{t_f} d\tau \left.\frac{\delta^2 S}{\delta x^2}\right|_{x=x_{xl}} \cdot y^2(\tau) + \cdots$$

Even if you are not familiar with functional differentiation, this is a rather easy step. Just replace $x \to x_{cl} + y$ in the Lagrangian and collect various powers of y (if need be, integrate by parts):

$$S[x_{cl}+y] = \int_{t_i}^{t_f} d\tau \left[\frac{m}{2}(\dot{x}_{cl}+\dot{y})^2 - V(x_{cl}+y)\right] = \int_{t_i}^{t_f} d\tau \left[\frac{m}{2}\dot{x}_{cl}^2 - V(x_{cl})\right]$$

$$+\int_{t_i}^{t_f} d\tau \left[m\dot{x}_{cl}\dot{y} - y\left.\frac{dV}{dx}\right|_{x=x_{cl}}\right] + \int_{t_i}^{t_f} d\tau \left[\frac{m}{2}\dot{y}^2 - \frac{y^2}{2}\left.\frac{d^2V}{dx^2}\right|_{x=x_{cl}} - \frac{y^3}{3!}\left.\frac{d^3V}{dx^3}\right|_{x=x_{cl}} - \ldots\right]$$

The first integral is just the action on the classical path, $S_{cl}(x_f,t_f;x_i,t_i)$. The second integral is zero, because integrating by parts it becomes equal to:

$$m\dot{x}_{cl}y\Big|_{t_i}^{t_f} - \int_{t_i}^{t_f} d\tau y(\tau)\left[m\ddot{x}_{cl} + \frac{dV}{dx_{cl}}\right]$$

The first term is zero because $y(t_i) = y(t_f) = 0$, and the second one because the classical trajectory satisfies the equation of motion $m\ddot{x}_{cl} = -\frac{dV}{dx_{cl}}$. It follows that:

$$\mathcal{G}(x_f,t_f;x_i,t_i) = e^{\frac{i}{\hbar}S_{cl}(x_f,t_f;x_i,t_i)}\int_{y(t_i)=0}^{y(t_f)=0}\mathcal{D}[y(\tau)]e^{\frac{i}{\hbar}\int_{t_i}^{t_f}d\tau\left[\frac{m}{2}\dot{y}^2-\frac{y^2}{2}\left.\frac{d^2V}{dx^2}\right|_{x=x_{cl}}-\frac{y^3}{3!}\left.\frac{d^3V}{dx^3}\right|_{x=x_{cl}}-\ldots\right]} \tag{1.52}$$

For the SHO, we can find the classical action by direct integration:

$$S_{cl}(x_f,t_f;x_i,t_i) = \int_{t_i}^{t_f} d\tau\left[\frac{m}{2}\dot{x}_{cl}^2 - \frac{k}{2}x_{cl}^2\right] = \frac{m\omega}{2\sin(\omega\Delta t)}\left[(x_i^2+x_f^2)\cos(\omega\Delta t) - 2x_ix_f\right]$$

Note: $S_{cl}(x_f,t_f;x_i,t_i)$ already gives a very non-trivial contribution to $\mathcal{G}$! In fact, for quadratic potentials, the entire dependence on x_i and x_f is here, the remaining term depends only on Δt. For more complicated potentials, the second term also depends on x_i and x_f.

Step 3 – The saddle-point approximation: we neglect all derivatives higher than $n = 2$ in the second term expansion, so that:

$$\mathcal{G}(x_f,t_f;x_i,t_i) \approx e^{\frac{i}{\hbar}S_{cl}(x_f,t_f;x_i,t_i)}\int_{y(t_i)=0}^{y(t_f)=0}\mathcal{D}[y(\tau)]e^{\frac{i}{\hbar}\int_{t_i}^{t_f}d\tau\left[\frac{m}{2}\dot{y}^2-\frac{y^2}{2}\left.\frac{d^2V}{dx^2}\right|_{x=x_{cl}}\right]} = e^{\frac{i}{\hbar}S_{cl}(x_f,t_f;x_i,t_i)}I \tag{1.53}$$

Note: for all quadratic potentials, those derivatives are identically zero so no approximation is involved. For higher order potentials we need to make this so-called saddle-point approximation.

Step 4: we now compute I, the final path integral. We first manipulate the exponent integrating by parts to obtain:

$$\int_{t_i}^{t_f} d\tau\left[\frac{m}{2}\dot{y}^2 - \frac{y^2}{2}\left.\frac{d^2V}{dx^2}\right|_{x=x_{cl}}\right] = -\frac{m}{2}\int_{t_i}^{t_f} d\tau y(\tau)\left[\frac{d^2}{d\tau^2} + \frac{1}{m}\left.\frac{d^2V}{dx^2}\right|_{x=x_{cl}}\right]y(\tau)$$

We now find the complete and orthonormal basis set for:

$$\left[\frac{d^2}{d\tau^2} + \frac{1}{m}\left.\frac{d^2V}{dx^2}\right|_{x=x_{cl}}\right]y_n(\tau) = \omega_n y_n(\tau)$$

with $y_n(t_i) = y_n(t_f) = 0$. Any cyclic path can be decomposed as $y(\tau) = \sum_n c_n y_n(\tau)$. Using the orthogonality $\int_{t_i}^{t_f} d\tau y_n(\tau) y_m(\tau) = \delta_{n,m}$, the integral in the exponent of I is simply:

$$-\frac{m}{2}\int_{t_i}^{t_f} d\tau y(\tau)\left[\frac{m}{2}\frac{d^2}{d\tau^2} + \frac{1}{2}\left.\frac{d^2V}{dx^2}\right|_{x=x_{cl}}\right] y(\tau) = -\frac{m}{2}\sum_n \omega_n c_n^2$$

At the same time, $\int \mathcal{D}[y(\tau)] \sim \prod_n \int_{-\infty}^{\infty} dc_n$, since considering all possible c_n values will cover all the possible cyclic paths. All the integrals are simple gaussians and we find:

$$I \sim \prod_n \frac{1}{\sqrt{\omega_n}} = \frac{1}{\sqrt{\det \sigma}}$$

where $\det \sigma = \prod_n \omega_n$. The elegant and easy way to compute this quantity is demonstrated in S. Coleman's *"Aspects of Symmetry"*, in Appedix 1. I summarize the solution here, but you should have a look at the proof. One has to find the solution $\phi(\tau)$ which satisfies:

$$\left[\frac{d^2}{d\tau^2} + \frac{1}{m}\left.\frac{d^2V}{dx^2}\right|_{x=x_{cl}}\right]\phi(\tau) = 0; \quad \phi(t_i) = 0; \quad \frac{d}{d\tau}\phi(t_i) = 1 \tag{1.54}$$

Then, $\det \sigma \sim \phi(t_f)$, and therefore collecting all terms, we find:

$$\mathcal{G}(x_f, t_f; x_i, t_i) \approx \frac{A}{\sqrt{\phi(t_f)}} e^{\frac{i}{\hbar} S_{cl}(x_f, t_f; x_i, t_i)} \tag{1.55}$$

and A is some normalization constant that may depend at most on Δt. The last step is to find A; this is done by requesting that in the limit $V \to 0$, $\mathcal{G} \to \mathcal{G}_0$ for the free particle, of Eq. (1.51).

Examples of computing $\det \sigma$:

(a) for free particle, $V = 0$. In this case, the classical action is trivial to find, $S_{cl} = \frac{m}{2\Delta t}(x_f - x_i)^2$. The solution of Eq. (1.54) is:

$$\frac{d^2}{d\tau^2}\phi(\tau) = 0 \to \phi(\tau) = a + b\tau$$

From the boundary conditions $\to a = -t_i, b = 1 \to \det \sigma \sim \phi(t_f) \sim \Delta t$ and so we find that:

$$\mathcal{G}_0(x_f, t_f; x_i, t_i) = \frac{A}{\sqrt{\Delta t}} e^{\frac{i}{\hbar}\frac{m}{2\Delta t}(x_f - x_i)^2}$$

which is the correct answer.

(b) for a SHO, $d^2V/dx^2 = k$, so Eq. (1.54) becomes:

$$\left(\frac{d^2}{d\tau^2} + \omega^2\right)\phi(\tau) = 0 \to \phi(\tau) = a\sin\omega(\tau - t_i) + b\cos\omega(\tau - t_i)$$

From the initial conditions, $b = 0, a = 1/\omega$ and so $\det \sigma \sim \phi(t_f) = \sin(\omega\Delta t)/\omega$. We thus find:

$$\mathcal{G}_{SHO}(x_f, t_f; x_i, t_i) = \sqrt{\frac{A\omega}{\sin(\omega\Delta t)}} e^{\frac{i}{\hbar}\frac{m\omega}{2\sin(\omega\Delta t)}\left[(x_i^2 + x_f^2)\cos(\omega\Delta t) - 2x_i x_f\right]}$$

Taking the limit $\omega \to 0$ (free particle) and requesting that $\mathcal{G}_{SHO} \to \mathcal{G}_0$, we find that $A = m/(2\pi i\hbar)$. The end result is:

$$\mathcal{G}_{SHO}(x_f, t_f; x_i, t_i) = \sqrt{\frac{m\omega}{2\pi\hbar i\sin(\omega\Delta t)}} e^{\frac{i}{\hbar}\frac{m\omega}{2\sin(\omega\Delta t)}\left[(x_i^2 + x_f^2)\cos(\omega\Delta t) - 2x_i x_f\right]} \tag{1.56}$$

$\mathcal{G}$ for any other quadratic potential can be calculated exactly in this manner; for higher order potentials, this approximation gives us a non-trivial (non-perturbational) expression for the propagator.

Before discussing the meaning of this saddle-point approximation, let us use the Feynman-Kac formula to extract the spectrum of the SHO from its propagator. Since:

$$\mathcal{G}(x_f,t_f;x_i,t_i)=\sum_n e^{-\frac{i}{\hbar}E_n\Delta t}u_n(x_f)u_n^*(x_i)\to\sum_n e^{-\frac{i}{\hbar}E_n\Delta t}=\int_{-\infty}^{\infty}dx\mathcal{G}(x,t_f;x,t_i)$$

Let us go to imaginary time, $\Delta t\to -iT$. Performing the gaussian integral, we now find:

$$\sum_n e^{-\frac{1}{\hbar}TE_n}=\sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega T)}}\int_{-\infty}^{\infty}dxe^{-\frac{1}{\hbar}\frac{m\omega}{2\sinh(\omega T)}2x^2[\cosh(\omega T)-1]}=\frac{e^{-\omega T/2}}{1-e^{-\omega T}}=\sum_{n=0}^{\infty}e^{-(n+1/2)\omega T}\to$$

$E_n=(n+1/2)\hbar\omega$. Which, of course, is exactly right.

1.7.2 The WKB approximation

As pointed out, S_{cl} already gives a rather non-trivial contribution to the propagator. Let us analyze its value for a potential barrier, such as sketched in Fig. 1.11. By definition, $\mathcal{G}(x_f,t_f;x_i,t_i)$ is the amplitude of probability that the particle will move from x_i to x_f, i.e. the transmission (tunneling) amplitude in this case. The energy of the particle on the classical trajectory is $E=\dot{x}\frac{\partial\mathcal{L}}{\partial\dot{x}}-\mathcal{L}=$

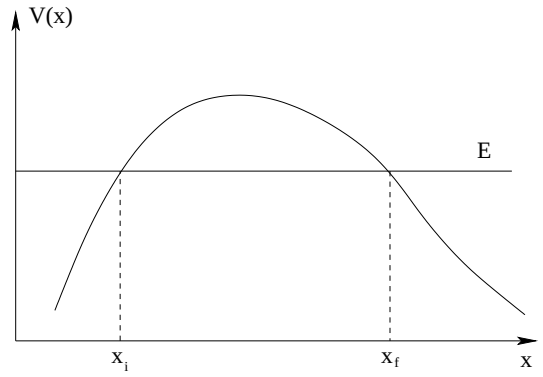

Figure 1.11: Tunneling barrier for a particle of energy E.

$\frac{m}{2}\dot{x}_{cl}^2+V(x_{cl})\to\dot{x}_{cl}=i\sqrt{2[V(x_{cl})-E]/m}$, since $E\le V(x_{cl})$ for $x\in[x_i,x_f]$. Also, along the classical trajectory, $\mathcal{L}=T-V=-E+2T$. Then, the classical action becomes:

$$S_{cl}(x_f,t_f;x_i,t_i)=\int_{t_i}^{t_f}d\tau\mathcal{L}=-E\Delta t+m\int_{t_i}^{t_f}d\tau\frac{dx_{cl}}{d\tau}\dot{x}_{cl}=-E\Delta t+i\int_{x_i}^{x_f}dx\sqrt{2m[V(x)-E]}$$

and therefore:

$$e^{\frac{i}{\hbar}S_{cl}}=e^{-\frac{i}{\hbar}E\Delta t}e^{-\frac{1}{\hbar}\int_{x_i}^{x_f}dx\sqrt{2m[V(x)-E]}}$$

The first term is just the usual time-dependent phase factor. The second term is the transmission amplitude in the WKB approximation. Finding a finite amplitude of probability to tunnel shows that this approximation is non-perturbative. In fact, for potentials higher than quadratic, the saddle-point approximation can be shown to be equivalent to the WKB approximation, i.e. $\mathcal{G}$ is calculated up to $\mathcal{O}(\hbar)$. Let us now consider a few more examples of path integrals.

1.7.3 The double-well potential – instantons

Let us assume a symmetric double-well potential, for instance:

$$V(x) = \frac{m\omega^2 a^2}{8}\left[1 - \frac{x^2}{a^2}\right]^2$$

This has up to x^4 terms, but we could deal with higher order terms in the same way. The coefficients were chosen so that $V_{min} = 0$ (an overall constant makes no difference) and the frequency of small oscillations about the minima $x = \pm a$ is ω. Since we did the SHO calculation for real time, let us do this for imaginary times, $\Delta t = -iT$. In this case [Eq. (1.50)]:

$$\mathcal{G}(x_f, -iT/2; x_i, iT/2) = \int \mathcal{D}[x(t)] e^{-\frac{1}{\hbar}\int_{\frac{-T}{2}}^{\frac{T}{2}} d\tau \left[\frac{m\dot{x}^2}{2} + V(x)\right]}$$

Clearly, we can use the method discussed in the last section if we replace in the exponents $i/\hbar \to -1/\hbar$ and change the sign of the potential. To make things even simpler, let $U(x) = -V(x)$, in which case:

$$\mathcal{G}(x_f, -iT/2; x_i, iT/2) = \int \mathcal{D}[x(t)] e^{-\frac{1}{\hbar}\int_{\frac{-T}{2}}^{\frac{T}{2}} d\tau \left[\frac{m\dot{x}^2}{2} - U(x)\right]}$$

and the "action" looks just as it did before, so we can apply the same formulas with U instead of V. The quantities we are really interested in are

$$\langle a | e^{-\frac{T}{\hbar}H} | \pm a \rangle$$

which contain the information about the amplitude of probability to tunnel or not to tunnel from one well to the other one. The first step is to find the classical action for the particle to move from a (at time $-T/2$) to $\pm a$ (at $T/2$), under the "potential" $U(x) = -V(x)$ shown in Fig. 1.12. Remember,

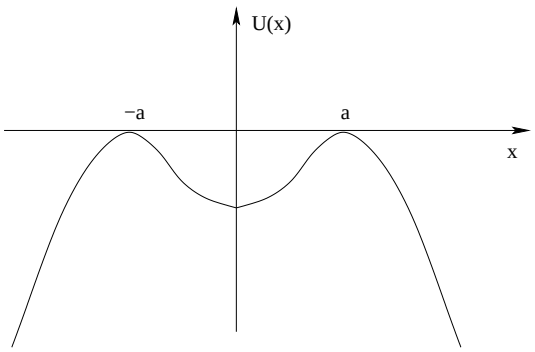

Figure 1.12: The "potential" $U(x) = -V(x)$.

we are now solving a classical problem. Clearly, the particle must have energy $E \geq 0$, otherwise it could not be at the $x = a$ to begin with. Moreover, we are interested in the limit $T \to \infty$ (which translates in low temperatures, since $T \sim \beta$, and thus will tell us something about the ground-state of the system). If the particle has energy $E > 0$, it goes towards $+\infty$ and never comes back (if it had a positive initial speed); or it will need a finite time to pass $-a$ and then keep moving towards $-\infty$, if it had initial negative speed. Obviously, the only way to have the particle at either $\pm a$ as $T \to \infty$ is if it has $E = 0$. Let us calculate first the classical action for the particle to be at $x = a$ at $T \to \infty$. For $E = 0$, we have several possible classical solutions:

i) the particle stays put at $x = a$ for all times $\rightarrow$ no contribution to action, since $\dot{x} = U(a) = 0$.

ii) particle makes a cycle $a \rightarrow -a \rightarrow a$, which is indeed possible for $E = 0$.

iii) particle makes two cycles $a \rightarrow -a \rightarrow a \rightarrow -a \rightarrow a$; etc.

There is an infinite number of solutions, each containing a different number of cycles. Similarly, if we want to find the classical action to move from a to $-a$, we again have an infinite number of solutions, and we have to consider all of them. Notice that all these solutions are made up of "pieces" where the particle moves from $x = -a$ at $t - T_0/2$, to $x = a$ at $t + T_0/2$ (or viceversa). So basically we need to find the classical action for this so called "instanton problem", and then sum together several instantons to obtain any of the trajectories described above.

Classical path for the instanton $(-a, t_0 - T_0/2) \rightarrow (+a, t_0 + T_0/2)$. From the conservation of energy:

$$E = 0 = \frac{m\dot{x}_{cl}^2}{2} + U(x_{cl}) \rightarrow 0 < \frac{dx_{cl}}{dt} = \sqrt{\frac{2}{m}[-U(x_{cl})]} \rightarrow t = t_0 + \int_0^x \frac{dx_{cl}}{\sqrt{\frac{2}{m}[-U(x_{cl})]}}$$

(the limits of the second integral are chosen using symmetry arguments. Of course, for an asymmetric potential, $t = t_0 - T/2 + \int_{-a}^{x} ...$). For the quartic potential we chose the integral can be performed exactly, and we find:

$$t = t_0 + \frac{2}{\omega} \tanh^{-1}\left(\frac{x}{a}\right) \rightarrow x_{cl}(t) = a \tanh \frac{\omega(t - t_0)}{2}$$

The instanton trajectory is shown in Fig. 1.13. Basically, the particle stays mostly at $-a$ or $+a$, except for an interval $\delta t \sim 1/\omega \ll T_0$ when it quickly moves from one position to the other one. By

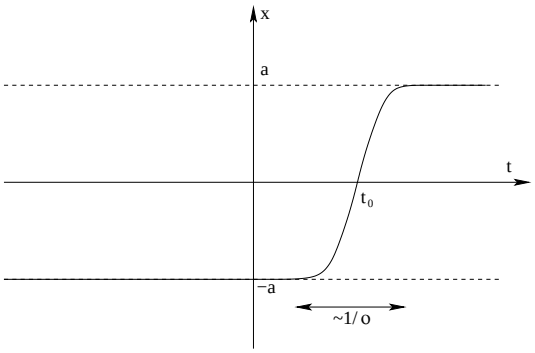

Figure 1.13: Instanton solution. The tunneling occurs over a timescale $1/\omega \ll T_0$ between consecutive tunnelings.

symmetry, the anti-instanton solution is:

$$x_{cl}(t) = -a \tanh \frac{\omega(t - t_0)}{2}$$

A typical trajectory that starts and ends in a is shown in Fig. 1.14. Each instanton is followed by an anti-instanton and viceversa, and since $T \rightarrow \infty$ we have $T \gg 1/\omega$ and therefore the instantons are essentially step functions at some times $-\frac{T}{2} < t_1 < t_2 < \ldots < t_{2N} < \frac{T}{2}$.

So, the first step is done: the classical trajectory for a curve such as the one in Fig. 1.14 is obtained by summing the proper series of instanton and anti-instanton solutions. The next step is to find the action for such a classical path. Since the contribution to the action from the regions where $x = a$ or $x = -a$ is zero, the total classical action will just the number of instantons plus antiinstantons,

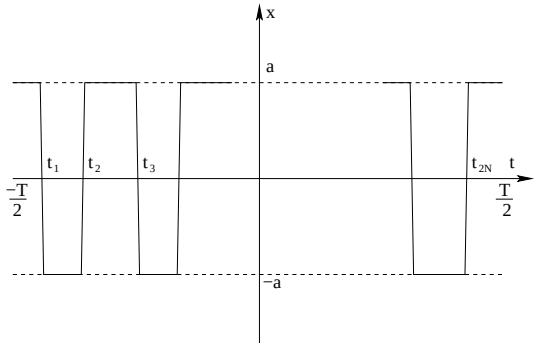

Figure 1.14: Classical trajectory $(a, \frac{-T}{2}) \to (a, \frac{T}{2})$ containing N instantons and N anti-instantons.

times the action for each of them. The action for each instanton (see the WKB discussion – after all, here we do have a particle of energy $E = 0$ tunneling through a barrier of potential $V(x)$) is:

$$S_{in} = \int_{-a}^{a} dx \sqrt{2m[V(x) - E]} = \frac{2}{3} m\omega^2 a^2$$

and therefore the classical action is nS_{in}, provided that $n/\omega \ll T$, i.e. the n instantons and anti-instantons do not overlap considerably (this is not likely to be a problem as $T \to \infty$, but one can demonstrate this more rigorously – again, see discussion in Coleman's book). The last part is to evaluate the path integral I over the cyclic trajectories (note that here we need to make the saddle-point approximation). For this we need to solve Eq. (1.54), where here we have:

$$\frac{1}{m} \left. \frac{d^2 U}{d^2 x} \right|_{x=x_{cl}} = -\frac{\omega^2}{2} \left[3\frac{x_{cl}^2(t)}{a^2} - 1 \right]$$

On any classical trajectory, most of the time $x_{cl} = \pm a$ and therefore the derivative is simply $-\omega^2$. Solving $(d^2/d\tau^2 - \omega^2)\phi(\tau) = 0, \phi(-T/2) = 0, d\phi/d\tau(-T/2) = 1 \to \phi(\tau) = \sinh[\omega(\tau + T/2)]/\omega \to 1/\sqrt{\det \sigma} \sim 1/\sqrt{\phi(T/2)} \sim \exp(-\omega T/2)$ as $T \to \infty$. If we have an instanton, we expect some correction to this value from the time interval where x changes from $-a$ to a. Let us call this correction K. In there are n instantons, there are n such time intervals in the exponent defining I – see Eq. (1.53), and therefore the correction should be K^n (to find K, we should solve Eq. (1.54) for the full instanton solution or use some other technique – see Coleman). The bottom line is that for n instantons, we expect

$$I \sim \frac{1}{\sqrt{\det \sigma}} \sim K^n e^{\frac{-\omega T}{2}}$$

We finally have all the ingredients. Remember that the propagator is the amplitude of probability for something to happen; if there are multiple ways we must sum over the amplitudes associated with all of them. We can have any number n of pairs of instantons and anti-instantons, and moreover they can occur at any times $-T/2 < t_1 < \ldots < t_{2n} < T/2$. As a result:

$$\langle a|e^{-\frac{T}{\hbar}H}|a\rangle = A \sum_{n=0}^{\infty} \int_{\frac{-T}{2}}^{\frac{T}{2}} dt_1 \int_{t_1}^{\frac{T}{2}} dt_2 \cdots \int_{t_{2n-1}}^{\frac{T}{2}} dt_{2n} e^{-\frac{1}{\hbar} 2nS_{in}} K^{2n} e^{-\frac{\omega T}{2}} = A e^{-\frac{\omega T}{2}} \sum_{n=0}^{\infty} \frac{1}{(2n)!} \left(K T e^{-\frac{S_{in}}{\hbar}} \right)^{2n}$$

where A is some proportionality constant. If we want the propagator for $a \to -a$, the only difference is that we have an odd number of instanton contributions, but otherwise things are very similar.

These series are well-known, and so:

$$\langle a|e^{-\frac{T}{\hbar}H}|\pm a\rangle = \frac{A}{2}e^{-\frac{\omega T}{2}}\left[e^{KTe^{-\frac{S_{in}}{\hbar}}} \pm e^{-KTe^{-\frac{S_{in}}{\hbar}}}\right] = \sum_n e^{-\frac{T}{\hbar}E_n}\langle a|n\rangle\langle n|\pm a\rangle$$

where $|n\rangle, E_n$ are the eigenstates and eigenenergies. In the limit $T\to\infty$, we find the two lowest eigenstates are:

$$E_\pm = \frac{\hbar\omega}{2} \pm \hbar K e^{-\frac{S_{in}}{\hbar}}$$

Indeed, the degeneracy between the two SHO ground-states associated with each well is lifted, and the splitting is proportional to the amplitude $\exp(-\frac{S_{in}}{\hbar})$ to tunnel through the barrier.

1.7.4 Particle coupled to a simple harmonic oscillator

We consider this problem here purely as an application for path integrals. However, it is worth pointing out that one often encounters such problems in solid state. For instance, an electron moving through a lattice of atoms at finite T will interact with the lattice vibrations (phonons), which can be modeled as simple harmonic oscillators.

Let us stay in 1D, for simplicity, and assume a single SHO. Let x be the particle coordinate, and X be the SHO coordinate. The propagator is the sum over histories, etc, so:

$$\mathcal{G} = \int \mathcal{D}[x(\tau)]\int \mathcal{D}[X(\tau)]e^{\frac{i}{\hbar}S[x,X]}$$

where the classical action is of the general form:

$$S = \int_{t_i}^{t_f} d\tau\left[\frac{m\dot{x}^2}{2} - V(x)\right] + \int_{t_i}^{t_f} d\tau\frac{M}{2}\left[\dot{X}^2 - \omega^2X^2\right] + \int_{t_i}^{t_f} d\tau g[x(\tau),\tau]X(\tau)$$

Here, the first term is the action for the particle of mass m, and the second is the action for the SHO of mass M and frequency ω. The last term representing their interaction is not quite as general as possible, instead we keep only a linear coupling. The idea is that the general interaction between the particle and the oscillator is some potential $V(x,X)$. The oscillator is assumed to vibrate close to its equilibrium position $X=0$ (otherwise, we would have to worry about unharmonic corrections and other complications). As a result, $V(x,X)\approx V(x,0) + XdV/dX|_{X=0} + \ldots$. The first term just contributes to the potential of the independent particle; the first interaction term is the linear coupling. For simplicity, we denote $g = dV/dX|_{X=0}$, and allow it to explicitly depend on time.

Note: the total action for the SHO is still quadratic and therefore we can do that path integral exactly! For simplicity, let us assume we are interested in the case $X_i = X_f = 0$, i.e. the SHO starts and ends in equilibrium. Then:

$$\mathcal{G}(x_f,t_f;x_i,t_i) = \int \mathcal{D}[x(\tau)]e^{\frac{i}{\hbar}S_{el}[x]}T[x]$$

where

$$T[x] = \int \mathcal{D}[X(\tau)]e^{\frac{i}{\hbar}\int_{t_i}^{t_f} d\tau\left[\frac{M}{2}\dot{X}^2 - \frac{M\omega^2}{2}X^2 + g[x(\tau),\tau]X\right]}$$

For any path $x(\tau)$, we have $g[x(\tau),\tau]$ is some overall function of τ. We follow the usual approach and expand this about its classical path, to obtain:

$$T[x] = e^{\frac{i}{\hbar}S_{cl}}\int_{Y(t_i)=0}^{Y(t_f)=0}\mathcal{D}[Y(\tau)]e^{\frac{i}{\hbar}\int_{t_i}^{t_f}\frac{M}{2}\left[\dot{Y}^2-\omega^2Y^2\right]}$$

Note: since the overall potential is quadratic in X, there is no approximation involved in this. Moreover, the linear coupling gives no contribution to the "cyclic" path integral over $Y = X - X_{cl}$, since only the second derivative of the potential appears in there [see Eq. (1.53)]. We have already calculated the path integral over Y in the SHO section. All we need to do is find the classical path for the SHO (which is influenced by the linear coupling, and can be found exactly) and the action associated with it. For $X_i = X_f = 0$, you should verify that the answer is:

$$T[x] = \sqrt{\frac{m\omega}{2\pi\hbar i \sin(\omega\Delta t)}} e^{\left(\frac{i}{\hbar m\omega \sin(\omega\Delta t)} \int_{t_i}^{t_f} dt_1 g[x(\tau_1),\tau_1] \sin[\omega(t_f - t_1)] \int_{t_i}^{t_f} dt_2 g[x(\tau_2),\tau_2] \sin[\omega(t_2 - t_i)]\right)}$$

One can also find this for the general case $X_i \neq 0$, $X_f \neq 0$, but the expression is rather long.

The amplitude of probability for the particle to move from x_i, t_i to x_f, t_f while the SHO starts and ends in equilibrium is, then:

$$\mathcal{G}(x_f, t_f; x_i, t_i) = \sqrt{\frac{m\omega}{2\pi\hbar i \sin(\omega\Delta t)}}$$

$$\times \int \mathcal{D}[x(\tau)] e^{\frac{i}{\hbar}\int_{t_i}^{t_f} d\tau \left[\frac{m\dot{x}^2}{2} - V(x)\right] + \frac{i}{\hbar m\omega \sin(\omega\Delta t)} \int_{t_i}^{t_f} dt_1 g[x(\tau_1),\tau_1] \sin[\omega(t_f - t_1)] \int_{t_i}^{t_f} dt_2 g[x(\tau_2),\tau_2] \sin[\omega(t_2 - t_i)]}$$

We can still say that $\mathcal{G} \sim \exp(\frac{i}{\hbar} S)$, but the "action" S is no longer simply the time integral of a Lagrangian, instead the new "effective interaction" term contains two time integrals. What this means is that we can no longer separate "past" and "future": the particle affects the oscillator at some time, and at some other time the oscillator reacts back and affects the particle. Integrating out the SHO is equivalent to introducing a non-local interaction of the particle with itself.

The main point of this exercise was to show that one can get quite easily a very non-trivial result, such as this non-local "effective interaction" that the electron feels when we average over the SHO. It is also quite trivial to generalize to having the particle interacting with as many SHO as we like, since the path integral over individual SHO coordinates are independent of one another. We could now wonder how to continue the calculation. If the coupling g is small, we could now expand in it, and stop at some reasonably high power. Even better, Feynman showed how one can estimate path integrals like this using a variational technique. This is nicely described in his book "Statistical Mechanics", in the "Polaron problem" chapter. Going through that calculation would make for a nice project. (Hopefully we'll have time to discuss more about the polarons later on). Another interesting topic, which should now be quite straightforward to tackle, is the famous Caldeira - Leggett work on the Brownian dynamics of a particle coupled to a bath of harmonic oscillators.

1.7.5 Coherent state representation

So far, we worked in the space representation. However, $|x\rangle$ is generally not the easiest basis in which to compute matrix elements and thus propagators, etc. Let us introduce a different basis, of so-called coherent states.

We start from a SHO Hamiltonian (1D):

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2}$$

and introduce the raising and lowering operators:

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + i\frac{\hat{p}}{m\omega}\right); \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - i\frac{\hat{p}}{m\omega}\right) \tag{1.57}$$

such that

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^\dagger\right); \qquad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\left(a^\dagger - a\right) \tag{1.58}$$

Properties (you should know this from a quantum mechanics course):

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

$$\hat{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$$

The eigenstates and eigenenergies $\hat{H}|n\rangle = E_n|n\rangle$, $n = 0, 1, 2, ...$ are:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle; \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

where

$$a|n\rangle = \sqrt{n}|n-1\rangle; \qquad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{1.59}$$

In the space representation, the eigenfunctions are:

$$\langle x|n\rangle = \sqrt{\frac{1}{\sqrt{\pi}l2^n n!}}e^{-\frac{x^2}{2l^2}}H_n\left(\frac{x}{l}\right) \tag{1.60}$$

where $H_n(x)$ are the Hermite polynomials, and

$$l = \sqrt{\frac{\hbar}{m\omega}} \tag{1.61}$$

is the characteristic length-scale.

Definition: the coherent states are the eigenstates of the non-Hermitian operator a: $a|z\rangle = z|z\rangle$, where $z \in C$ is any complex number.

Since $|n\rangle$ form a complete basis set, $|z\rangle = \sum_n \alpha_n|n\rangle$. From $a|z\rangle = z|z\rangle \to \alpha_{n+1} = \alpha_n z/\sqrt{n+1} = \ldots = \alpha_0 z^{n+1}/\sqrt{(n+1)!}$. Thus, up to some normalization factor which we will call $N(z)$, we have:

$$|z\rangle = N(z)\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\left(\frac{a^n}{\sqrt{n!}}|0\rangle\right) = N(z)e^{za^\dagger}|0\rangle \tag{1.62}$$

The choice for $N(z)$ is not unique. Sometimes it is convenient to take $N(z) = 1$. For the time being, let us choose is such that $|z\rangle$ are normalized. In fact, let us calculate

$$\langle z'|z\rangle = N^*(z')N(z)\langle 0|e^{z'^* a}e^{za^\dagger}|0\rangle$$

We use the Baker-Hausdorff identity $e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$, which holds provided that $[A,[A,B]] = [B,[A,B]] = 0$. For us $A = z'^* a, B = za^\dagger \to [A,B] = z'^* z$. Using the identity twice, we have $e^A e^B = e^B e^A e^{[A,B]}$, and since $\langle 0|e^{za^\dagger}e^{z'^* a}|0\rangle = 1$, we find that $\langle z'|z\rangle = N^*(z')N(z)\exp(z'^* z)$. From $\langle z|z\rangle = 1 \to N(z) = \exp(-|z|^2/2)$. Thus, we will use the normalization:

$$|z\rangle = e^{-\frac{|z|^2}{2}+za^\dagger}|0\rangle \to \langle z'|z\rangle = e^{z'^* z - \frac{|z|^2}{2} - \frac{|z'|^2}{2}} \tag{1.63}$$

Note: the coherent states are *not* orthogonal to one another!

Before continuing, let us see the meaning of these coherent states. Using Eq. (1.58), we find that

$$\bar{x}_z = \langle z|\hat{x}|z\rangle = \sqrt{2}l\mathrm{Re}z; \qquad \bar{p}_z = \langle z|\hat{p}|z\rangle = \frac{\hbar}{\sqrt{2}l}\mathrm{Im}z \rightarrow z = \frac{\bar{x}_z}{\sqrt{2}l} + i\frac{l}{\sqrt{2}\hbar}\bar{p}_z$$

This last equality is very suggestive: the real part of z is related to the position expectation value, and its imaginary part is related to the momentum expectation value [see also Eq. (1.57)]. One can similarly calculate (verify!):

$$\langle z|\hat{x}^2|z\rangle = \frac{l^2}{2}\left(1+2|z|^2+z^2+z^{*2}\right);\ \ \langle z|\hat{p}^2|z\rangle = \frac{\hbar^2}{2l^2}\left(1+2|z|^2-z^2-z^{*2}\right) \rightarrow \langle z|\hat{H}|z\rangle = \hbar\omega(|z|^2+1/2)$$

More importantly,

$$\Delta x_z = \sqrt{\langle z|\hat{x}^2|z\rangle - \langle z|\hat{x}|z\rangle^2} = \frac{l}{\sqrt{2}}; \quad \Delta p_z = \sqrt{\langle z|\hat{p}^2|z\rangle - \langle z|\hat{p}|z\rangle^2} = \frac{\hbar}{\sqrt{2}l} \rightarrow \Delta x_z \Delta p_z = \frac{\hbar}{2}$$

The coherent states are minimum uncertainty wave packets!. What do they look like in the x-representation? Assignment:

$$\langle x|z\rangle = \sqrt{\frac{1}{\sqrt{\pi}l}}e^{-\frac{(x-\bar{x}_z)^2}{2l^2}+\frac{i}{\hbar}\bar{p}_z x-\frac{i}{2\hbar}\bar{p}_z\bar{x}_z}$$

In other words, a gaussian centered at $\bar{x}_z$ (no surprise), "smeared out" over a distance l (this "smearing" explains why different coherent states are not orthogonal to one another). It also has oscillating behavior with the average momentum $\bar{p}_z$.

How about time evolution?

$$e^{-\frac{i}{\hbar}\hat{H}t}|z\rangle = e^{-\frac{|z|^2}{2}}\sum_n \frac{z^n}{\sqrt{n!}}e^{-i\omega(n+1/2)t}|n\rangle = e^{-\frac{i\omega t}{2}}|ze^{-i\omega t}\rangle$$

i.e. we just get a different coherent state. Then (assignment!):

$$\langle x|e^{-\frac{i}{\hbar}\hat{H}t}|z\rangle = \sqrt{\frac{e^{-i\omega t}}{\sqrt{\pi}l}}e^{-\frac{(x-\bar{x}_z(t))^2}{2l^2}+\frac{i}{\hbar}\bar{p}_z(t)x-\frac{i}{2\hbar}\bar{p}_z(t)\bar{x}_z(t)}$$

where

$$\bar{x}_z(t) = \bar{x}_z\cos(\omega t) + \frac{\bar{p}_z}{m\omega}\sin(\omega t); \quad \bar{p}_z(t) = \bar{p}_z\cos(\omega t) - m\omega\bar{x}_z\sin(\omega t)$$

All these equations look very reasonable.

One last essential thing we need is the resolution of identity, i.e. the equivalent of $\int dx|x\rangle\langle x| = 1$. The set of coherent states $\{|z\rangle|z\in C\}$ is complete: any state can be written as a linear combination of coherent states. However, the set is *overcomplete* (e.g., show that $\int d^2z z|z\rangle = 0$). This should not be too shocking, since we know that the basis $\{|n\rangle|n\in N\}$ is complete, and there are many more $|z\rangle$ states than $|n\rangle$ states. Because of overcompletness, the resolution of identity is not unique. We will use the formula:

$$\int \frac{d^2z}{\pi}|z\rangle\langle z| = 1 \tag{1.64}$$

where $d^2z = d(\mathrm{Re}z)d(\mathrm{Im}z)$.

Proof:

$$\int \frac{d^2z}{\pi}|z\rangle\langle z| = \sum_{n,m}\frac{|n\rangle\langle m|}{\sqrt{n!m!}}\int\frac{d^2z}{\pi}e^{-|z|^2}z^{*n}z^m = \text{(in polar coordinates)}$$

$$= \sum_{n,m} \frac{|n\rangle\langle m|}{\sqrt{n!m!}} \int_0^\infty d\rho \rho^{1+n+m} e^{-\rho^2} \frac{1}{\pi} \int_0^{2\pi} d\phi e^{i(m-n)\phi} = 2 \sum_n \frac{|n\rangle\langle n|}{n!} \int_0^\infty d\rho \rho^{2n+1} e^{-\rho^2} = \sum_n |n\rangle\langle n| = 1$$

Hopefully, you are by now convinced that it is fairly easy to compute matrix elements over coherent states. As a final proof, let us compute the propagator for the SHO oscillator using coherent states.

The amplitude of probability to go from z_i, t_i to z_f, t_f is quite trivial:

$$\mathcal{G}(z_f, t_f; z_i, t_i) = \langle z_f | e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} | z_i \rangle = e^{-\frac{i\omega\Delta t}{2}} \langle z_f | z_i e^{-i\omega\Delta t} \rangle = e^{-\frac{i\omega\Delta t}{2}} e^{-\frac{1}{2}(|z_i|^2 + |z_f|^2) + z_f^* z_i e^{-i\omega\Delta t}}$$

More interesting is to check the SHO propagator we obtained previously, in x-representation. Using Eq. (1.64), we have:

$$\mathcal{G}(x_f, t_f; x_i, t_i) = \langle x_f | e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} | x_i \rangle = \int \frac{d^2 z}{\pi} \langle x_f | z \rangle \langle z | e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} | x_i \rangle$$

We've already calculated these matrix elements before. After a bit of work, the exponent can be written as a sum of quadratic forms in $\bar{x}_z$ and $\bar{p}_z$, which, remember, are proportional to Rez and Imz, and therefore are the variables of integration. The gaussian integrals are straightforward, and – no surprise – we get the correct result rather trivially. You should check this!

More interesting is how we use coherent states to compute the propagators for other (not SHO) Hamiltonians. We discuss this next.

1.7.6 Coherent-state representation for path integrals

Since we have

$$\mathcal{G}(x_f, t_f; x_i, t_i) = \int \frac{d^2 z_i}{\pi} \int \frac{d^2 z_f}{\pi} \langle x_f | z_f \rangle \mathcal{G}(z_f, t_f; z_i, t_i) \langle z_i | x_i \rangle,$$

if we know $\mathcal{G}(z_f, t_f; z_i, t_i) = \langle z_f | e^{-\frac{i}{\hbar}\hat{H}\Delta t} | z_i \rangle$ (remember, the $\Theta(t_f - t_i)$ is implied) then we can calculate the x-space (or any other) representation of the propagator. To calculate $\mathcal{G}(z_f, t_f; z_i, t_i)$ we will proceed exactly as before: we divide the time interval into N equal subintervals of length $\epsilon = \Delta t/N$; we write the exponential as a product of N exponentials, and insert $N-1$ resolutions of identity in between. As before, we denote $z_0 \equiv z_i$, $z_N \equiv z_f$. At this stage, we have:

$$\mathcal{G}(z_f, t_f; z_i, t_i) = \lim_{N\to\infty} \int \frac{d^2 z_1}{\pi} \cdots \int \frac{d^2 z_{N-1}}{\pi} \prod_{j=1}^{N} \langle z_j | e^{-\frac{i}{\hbar}\epsilon\hat{H}} | z_{j-1} \rangle$$

Now we need to evaluate the matrix elements. For $\epsilon \ll 1$, we have:

$$\langle z_j | e^{-\frac{i}{\hbar}\epsilon\hat{H}} | z_{j-1} \rangle \approx \langle z_j | 1 - \frac{i}{\hbar}\epsilon\hat{H} | z_{j-1} \rangle + \mathcal{O}(\epsilon^2) \approx \langle z_j | z_{j-1} \rangle e^{-\frac{i}{\hbar}\epsilon H(z_j^*, z_{j-1})} + \mathcal{O}(\epsilon^2)$$

where, *by definition*:

$$H(\alpha^*, \beta) = \frac{\langle \alpha | \hat{H} | \beta \rangle}{\langle \alpha | \beta \rangle} \tag{1.65}$$

and can be calculated once we are given $\hat{H}$. The overlap is:

$$\langle z_j | z_{j-1} \rangle = e^{-\frac{1}{2}(|z_j|^2 + |z_{j-1}|^2) + z_j^* z_{j-1}} = e^{-\frac{\epsilon}{2}[z_j^* \frac{z_j - z_{j-1}}{\epsilon} - \frac{z_j^* - z_{j-1}^*}{\epsilon} z_{j-1}]}$$

Thus, we now have:

$$\mathcal{G}(z_f,t_f;z_i,t_i)=\lim_{N\to\infty}\int\frac{d^2z_1}{\pi}\cdots\int\frac{d^2z_{N-1}}{\pi}e^{\frac{i}{\hbar}\sum_{j=1}^{N}\epsilon\left[\frac{i\hbar}{2}\left(z_j^*\frac{z_j-z_{j-1}}{\epsilon}-\frac{z_j^*-z_{j-1}^*}{\epsilon}z_{j-1}\right)-H(z_j^*,z_{j-1})\right]}$$

The sum in the exponent can be transformed into an integral, and using the notation:

$$\frac{z_j-z_{j-1}}{\epsilon}=\frac{dz}{d\tau}$$

we finally have:

$$\mathcal{G}(z_f,t_f;z_i,t_i)=\int_{z(t_i)=z_i}^{z(t_f)=z_f}\mathcal{D}[z(\tau)]e^{\frac{i}{\hbar}\int_{t_i}^{t_f}d\tau\left[\frac{i\hbar}{2}\left(z^*\frac{dz}{d\tau}-\frac{dz^*}{d\tau}z\right)-H(z^*(\tau),z(\tau))\right]}\tag{1.66}$$

For many-body bosonic systems, the path-integrals will look exactly like this one, except that each species of bosons will have its own coherent variable, $a_\alpha|z_\alpha\rangle=z_\alpha|z_\alpha\rangle$. In the first term in the action we will then sum over all modes: $\int_{t_i}^{t_f}d\tau\sum_\alpha\left[\frac{i\hbar}{2}\left(z_\alpha^*\frac{dz_\alpha}{d\tau}-\frac{dz_\alpha^*}{d\tau}z_\alpha\right)\right]=i\hbar\int_{t_i}^{t_f}d\tau\sum_\alpha z_\alpha^*\frac{dz_\alpha}{d\tau}$ (up to a term that depends only on the initial and final norms of the various z_α). The generalization for the second term is also straightforward. Computing the expression of $H(\{z_\alpha^*\},\{z_\alpha\})$ is especially simple if the Hamiltonian is in "normal order", which means that all creation operators are at the left of all annihilation operators. For instance, consider a 2-boson Hamiltonian:

$$\mathcal{H}=\epsilon_1a_1^\dagger a_1+\epsilon_2a_2^\dagger a_2+u_1\hat{n}_1\hat{n}_1+u_2\hat{n}_2\hat{n}_2+u\hat{n}_1\hat{n}_2$$

where $\hat{n}_1=a_1^\dagger a_1,\hat{n}_2=a_2^\dagger a_2$. The last 3 terms describe interactions between bosons of type 1 and 2 with themselves and the other specie. Terms like $\hat{n}_1\hat{n}_1=a_1^\dagger a_1a_1^\dagger a_1$ are not normally ordered, but that is trivial to do since $aa^\dagger=a^\dagger a+1$ for each species, while different species commute, so that:

$$\mathcal{H}=(\epsilon_1+u_1)a_1^\dagger a_1+(\epsilon_2+u_2)a_2^\dagger a_2+u_1a_1^\dagger a_1^\dagger a_1a_1+u_2a_2^\dagger a_2^\dagger a_2a_2+ua_1^\dagger a_2^\dagger a_1a_2$$

Evaluating the expectation values in the coherent basis is now trivial:

$$H(z_1^*,z_2^*,z_1,z_2)=\frac{\langle z_1,z_2|\mathcal{H}|z_1,z_2\rangle}{\langle z_1,z_2|z_1,z_2\rangle}=(\epsilon_1+u_1)|z_1|^2+(\epsilon_2+u_2)|z_2|^2+u_1|z_1|^4+u_2|z_2|^4+u|z_1|^2|z_2|^2$$

Note: the reason I keep dividing by $\langle z|z\rangle$, although we work with normalized states, is to remind you that in case you choose non-normalized coherent states (which is quite customary, e.g. Negele and Orland) then you have to be a bit careful.

One more note: for fermionic systems, one can do very similar tricks – define coherent states and express the path integrals in terms of coherent variables, with expressions that look very similar to what we have above. However, there is an essential difference: fermionic operators anticommute, and we somehow need to take that into consideration. For instance, if $a_1|z_1,z_2\rangle=z_1|z_1,z_2\rangle$ and $a_2|z_1,z_2\rangle=z_2|z_1,z_2\rangle$ is a coherent state for two fermionic annihilation operators, then since $a_1a_2=-a_2a_1$, we must have $z_1z_2=-z_2z_1$. So these numbers cannot be the usual complex numbers, but something else. They are so-called Grassman variables, and they simply satisfy some such funny rules to insure proper statistics, but other than that there's nothing complicated about them. Hopefully we'll get to discuss this later on (although last year I ran out of time). If not, these issues are very nicely discussed in the first 2 chapters of Orland and Negele. I think you now have enough background to be able to read through that on your own (project topic?).

Let me go back to the single boson discussion, and Eq. (1.66). We expect that the exponent is an "action". Let us see what equations of motion we could derive from this action.

Let

$$z = \frac{1}{\sqrt{2}}(\xi + i\pi)$$

where, remember, $\xi = \bar{x}_z/l$ is related to the expectation value of the position operator of the particle, in dimensionless units, and similarly $\pi = l\bar{p}_z/\hbar$ is related to the average momentum of the particle in the state $|z\rangle$. Then,

$$z^* \frac{dz}{d\tau} - \frac{dz^*}{d\tau} z = -i\pi\dot{\xi} + i\dot{\pi}\xi$$

and the action is:

$$S = \int_{t_i}^{t_f} d\tau \left[\frac{\hbar}{2}\left(\pi\dot{\xi} - \dot{\pi}\xi\right) - h(\xi,\pi)\right]$$

where

$$h(\xi,\pi) = H\left(\frac{\xi - i\pi}{\sqrt{2}}, \frac{\xi + i\pi}{\sqrt{2}}\right)$$

Requesting that $\delta S = 0$, after two integrations by parts, we find the equations of motion:

$$\hbar\dot{\xi} = \frac{\partial h}{\partial \pi}; \qquad \hbar\dot{\pi} = -\frac{\partial h}{\partial \xi}$$

which are just the analog of Hamilton's equations.

Finally, let us also give the finite-temperature version. In this case, $\Delta t \to -i\hbar\beta$ and, for instance, the partition function is:

$$Z = \sum_n e^{-\beta E_n} = \int \frac{d^2z}{\pi} \langle z|e^{-\beta\hat{H}} \sum_n |n\rangle\langle n|z\rangle = \int \frac{d^2z}{\pi} \langle z|e^{-\beta\hat{H}}|z\rangle.$$

The integrand is a "cyclic" propagator, so we need to sum over all paths for which $z(0) = z(\beta)$ to find:

$$Z = \int_{z(0)=z(\beta)} \mathcal{D}[z(\tau)] e^{-\int_0^\beta d\tau \left[\frac{1}{2}\left(z^*\frac{dz}{d\tau} - \frac{dz^*}{d\tau}z\right) + H(z^*(\tau), z(\tau))\right]} \tag{1.67}$$

1.8 Path integral for a spin

Strictly speaking, this should be discussed in a course on magnetism. However, we briefly look at it here, for completeness and also to emphasize that the general philosophy behind the path-integral formulation is the same, no matter what system we consider.

We move to the opposite extreme of the case we discussed before, and assume that our particle has only spin degrees of freedom (it is localized in real space). Its Hamiltonian, then, is of the form:

$$\hat{H}(t) = -g\mu_B \hat{\vec{S}} \cdot \vec{B}(t) = -\hat{\vec{S}} \cdot \vec{h}(t) \tag{1.68}$$

where $\vec{h}$ is the external magnetic field in renormalized units. From all we've discussed so far, we expect that:

$$\hat{\mathcal{G}}(t_f, t_i) = \Theta(t_f - t_i)\mathbf{T} e^{-\frac{i}{\hbar}\int_{t_i}^{t_f} d\tau \hat{H}(\tau)} \to \sum_{\text{all paths}} e^{\frac{i}{\hbar}S}$$

where S is the classical action associated with the different paths. At this point it should be clear that we'll have some difficulties, because:

i) the usual basis for a spin S is $\{|S,m\rangle|m=-S,...,S\}$ which is $2S+1$ -dimensional. For simplicity, from now on we do not write S explicitly, since it is fixed, so $|S,m\rangle \equiv |m\rangle$, and the resolution of identity is $\sum_{m=-S}^{S}|m\rangle\langle m| = 1$. The problem is that this is a discrete basis, we cannot use it to define "continuous" paths $m(\tau)$ the way we had paths $x(\tau)$ before.

ii) the spin has no classical analog, because in the limit $\hbar \to 0$ the spin expectation values go to zero, since $\hat{S}_z|m\rangle = \hbar m|m\rangle$ etc. You might argue that this is not a correct statement, since the angular momentum has similar eigenstates as the spin operator, namely $\hat{\vec{L}}|L,M\rangle = \hbar^2 L(L+1)|L,M\rangle; \hat{L}_z|L,M\rangle = \hbar M|L,M\rangle$. However, here there is no problem in letting $\hbar \to 0$ because we can let $L \to \infty$ (macroscopic classical objects have large angular momenta). We can't do the same for a spin, since S is fixed. The bottom line is that there is no "classical action" for a spin and formulating the path-integral formulation is not obvious – in fact, Feynman could not figure it out. The solution is actually very neat and interesting, and ties well with what we discussed so far, as we will see. The first thing we need is another (obviously overcomplete) basis, which must be characterized by quantities that vary continuously. In effect, we need a coherent state representation for spins.

1.8.1 Spin coherent states

Any rotation is spin space can be parameterized by 3 Euler angles, χ, θ, ϕ. **Note:** we use the convention that we rotate the object (not the system of coordinates) anti-clockwise. The series of transformations characterizing an overall rotation are: (1) a rotation by angle χ about $0z$ axis; (2) a rotation by θ about the Oy axis, and (3) a rotation by ϕ about the $0z$ axis. Choosing properly χ, θ, ϕ we can take a spin oriented along the z-axis and rotate it to any desired position, as shown in Fig. 1.15. **Note:** in this case, the first rotation is just a gauge transformation, we can always choose the orientation of the xOy axes so as to eliminate it.

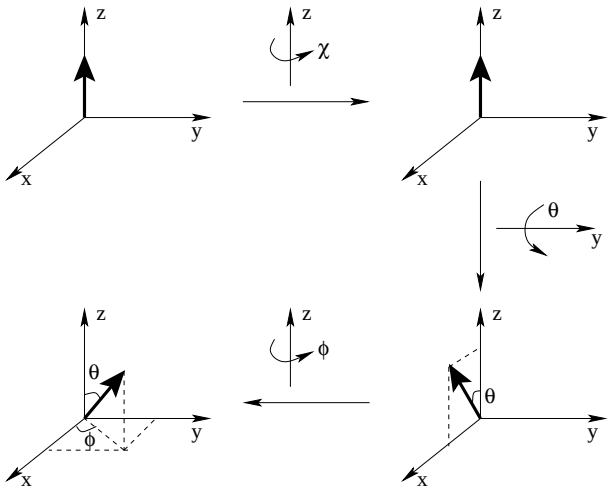

Figure 1.15: The 3 Euler rotations that take the spin from Oz orientation to any desired state.

The operator for clockwise rotation by angle α about axis i is:

$$\hat{R}_i(\alpha) = e^{-\frac{i}{\hbar}\hat{S}_i\alpha} \tag{1.69}$$

For example, you should check that $\hat{R}_z(\phi)\hat{S}_x\hat{R}_z^\dagger(\phi) = \hat{S}_x\cos\phi + \hat{S}_y\sin\phi$, i.e. indeed the spin pointing along $0x$ has been rotated anticlockwise by ϕ about the $0z$ axis. For this, show that

$$F(\lambda) = e^{-\lambda A}Be^{\lambda A} = \sum_{n\geq 0}\frac{\lambda^n}{n!}\frac{d^nF}{d\lambda^n}|_{\lambda=0} = \sum_n \frac{\lambda^n}{n!}[....[[B,A],A]...,A]$$

where we have n commutators in the expression. For spin operators those multiple commutators can be evaluated easily.

The operator describing the rotations shown in Fig. 1.15 is:

$$\hat{R}(\chi,\theta,\phi) = e^{-\frac{i}{\hbar}\phi\hat{S}_z}e^{-\frac{i}{\hbar}\theta\hat{S}_y}e^{-\frac{i}{\hbar}\chi\hat{S}_z} \tag{1.70}$$

Indeed, we have:

$$\hat{R}(\chi,\theta,\phi)\hat{S}_z\hat{R}^\dagger(\chi,\theta,\phi) = \hat{S}_x\sin\theta\cos\phi + \hat{S}_y\sin\theta\sin\phi + \hat{S}_z\cos\theta = \hat{\vec{S}}\cdot\vec{\Omega} \tag{1.71}$$

where $\vec{\Omega} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is the unit vector for the final orientation of the rotated spin (see Fig. 1.15). **Note:** there are several ways in which to define the Euler rotations (for instance, the second one could be about the Ox axis, or one could rotate the spins clockwise or – equivalently – the system of coordinates anti-clockwise. In this section we will stick with these definitions, which might differ by the sign in the phase from definitions you see in other places. As long as the convention doesn't change midway through the calculation, we will get the correct result.

Definition: the spin coherent state

$$|\vec{\Omega}\rangle = \hat{R}(\chi,\theta,\phi)|S,+S\rangle \tag{1.72}$$

Then,

$$\left(\hat{\vec{S}}\cdot\vec{\Omega}\right)|\vec{\Omega}\rangle = \left(\hat{R}\hat{S}_z\hat{R}^\dagger\right)\hat{R}|S,+S\rangle = \hbar S|\vec{\Omega}\rangle$$

in other words, $|\vec{\Omega}\rangle$ is *the state with maximum spin projection along the* $\vec{\Omega}$ *axis*. Clearly, these states are very promising since we can easily envision continuous paths $\vec{\Omega}(\tau)$! As for the coherent states discussed before, we now need to be able to compute their overlap, and find a resolution of identity. To do this fairly easily, we will use the Schwinger representation for spins.

1.8.2 Schwinger bosons

We introduce two bosonic operators a and b such that:

$$\hat{S}_+ = \hat{S}_x + i\hat{S}_y = \hbar a^\dagger b; \quad \hat{S}_- = \hat{S}_x - i\hat{S}_y = \hbar b^\dagger a; \quad \hat{S}_z = \frac{\hbar}{2}\left(a^\dagger a - b^\dagger b\right) \tag{1.73}$$

It is straightforward to check that the spins satisfy the proper commutation $[\hat{S}_\alpha, \hat{S}_\beta] = i\hbar\epsilon_{\alpha\beta\gamma}\hat{S}_\gamma$. A general eigenstates of $\hat{S}_z$ is of the form:

$$|n_a,n_b\rangle = \frac{(a^\dagger)^{n_a}}{\sqrt{n_a!}}\frac{(b^\dagger)^{n_b}}{\sqrt{n_b!}}|0\rangle \rightarrow \hat{S}_z|n_a,n_b\rangle = \frac{\hbar}{2}(n_a-n_b)|n_a,n_b\rangle$$

where here $|0\rangle$ is the bosonic vacuum, and $n_a, n_b = 0,1,2,....$ These vectors generate an infinite number of states, of which only $2S+1$ are physical. Let's identify them. Firstly,

$$\hat{S}_+|n_a,n_b\rangle = \sqrt{(n_a+1)n_b}|n_a+1,n_b-1\rangle; \quad \hat{S}_-|n_a,n_b\rangle = \sqrt{n_a(n_b+1)}|n_a-1,n_b+1\rangle$$

so $n_a + n_b = $ const. in the physical subspace. Moreover, we can only apply the lowering or raising operator at most $2S$ times, and therefore we must have $n_a + n_b = 2S$. But $n_a - n_b = 2m$ (see eigenvalue of $\hat{S}_z$), and so the values $n_a = S + m, n_b = S - m$, $m = -S, ..., S$ span the physical subspace, and:

$$|S, m\rangle = \frac{(a^\dagger)^{S+m}}{\sqrt{(S+m)!}} \frac{(b^\dagger)^{S-m}}{\sqrt{(S-m)!}} |0\rangle \tag{1.74}$$

What is the effect of performing a rotation $\hat{R}(\chi, \theta, \phi)$ on the Schwinger operators? We must obtain two new operators, a' and b', linked to the old ones through some general unitary transformation:

$$RaR^\dagger = a' = ua + vb; \quad RbR^\dagger = b' = -v^* a + u^* b;$$

where $|u|^2 + |v|^2 = 1$ are some complex numbers. Then:

$$\hat{\vec{S}} \cdot \vec{\Omega} = RS_z R^\dagger = R\frac{\hbar}{2}\left(a^\dagger a - b^\dagger b\right) R = \frac{\hbar}{2}\left(a'^\dagger a' - b'^\dagger b'\right) = [|u|^2 - |v|^2]\hat{S}_z + u^* v \hat{S}_+ + u v^* \hat{S}_-$$

From Eq. (1.71) it follows that we must have $|u|^2 - |v|^2 = \cos\theta$, etc, so the general solution is

$$u = \cos\frac{\theta}{2} e^{i\alpha}; \quad v = \sin\frac{\theta}{2} e^{i\beta}$$

where $\alpha - \beta = \phi$. The rotation by χ is a simple gauge transformation, and we will choose $\alpha + \beta = -\chi$ (at this point, we could choose anything, but later we'll show that this is the proper choice). This fixes the values of u and v uniquely, and so the rotated Schwinger operators are:

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} e^{i\frac{\phi-\chi}{2}} & \sin\frac{\theta}{2} e^{-i\frac{\phi+\chi}{2}} \\ -\sin\frac{\theta}{2} e^{i\frac{\phi+\chi}{2}} & \cos\frac{\theta}{2} e^{-i\frac{\phi-\chi}{2}} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \tag{1.75}$$

We can now finally write the spin coherent state in terms of Schwinger operators:

$$|\vec{\Omega}\rangle = \hat{R}|S, +S\rangle = \hat{R}\frac{(a^\dagger)^{2S}}{\sqrt{(2S)!}}|0\rangle = \frac{(u^* a^\dagger + v^* b^\dagger)^{2S}}{\sqrt{(2S)!}}|0\rangle$$

and therefore find their decomposition in the $|S, m\rangle$ basis:

$$|\vec{\Omega}\rangle = e^{-iS\chi}\sqrt{(2S)!} \sum_{m=-S}^{S} \frac{[\cos\frac{\theta}{2}]^{S+m}[\sin\frac{\theta}{2}]^{S-m}}{\sqrt{(S+m)!(S-m)!}} e^{-im\phi}|S, m\rangle \tag{1.76}$$

Note: this expression is quite reasonable, since by definition $|\vec{\Omega}\rangle = e^{-\frac{i}{\hbar}\phi\hat{S}_z} e^{-\frac{i}{\hbar}\theta\hat{S}_y} e^{-\frac{i}{\hbar}\chi\hat{S}_z}|S, +S\rangle$. The first operator gives the $e^{-iS\chi}$ term in Eq. (1.76) – this is actually why choosing the phases of u and v such that $\alpha + \beta = -\chi$ is the correct choice. The second operator's action on $|S, +S\rangle$ mixes in all components $|S, m\rangle$, because $\hat{S}_y = (1/2i)(\hat{S}_+ - \hat{S}_-)$. Finally, the third operator acting on any $|S, m\rangle$ gives the $e^{-im\phi}$ phase. So the expression is reasonable, the only question was how to find the coefficients, and use of the Schwinger bosons gives us one of the more elegant ways to do it.

We can now use Eq. (1.76) to find the overlap of two spin coherent states:

$$\langle\vec{\Omega}_1|\vec{\Omega}_2\rangle = e^{-iS(\chi_2-\chi_1)}(2S)! \sum_{m=-S}^{S} \frac{[\cos\frac{\theta_1}{2}\cos\frac{\theta_2}{2} e^{i\frac{\phi_1-\phi_2}{2}}]^{S+m}[\sin\frac{\theta_1}{2}\sin\frac{\theta_2}{2} e^{-i\frac{\phi_1-\phi_2}{2}}]^{S-m}}{(S+m)!(S-m)!} = \left(\frac{1 + \vec{\Omega}_1 \cdot \vec{\Omega}_2}{2}\right)^{2S} e^{-iS\psi} \tag{1.77}$$

where $\psi = \chi_2 - \chi_1 - 2\tan^{-1}\left(\tan\frac{\phi_1-\phi_2}{2}\cos\frac{\theta_1+\theta_2}{2}\cos^{-1}\frac{\theta_1-\theta_2}{2}\right)$. This shows that the spin coherent states are not orthogonal to one another, instead the closer the two vectors $\vec{\Omega}_1$ and $\vec{\Omega}_2$ are to one another, the larger is the overlap.

Since the set of spin coherent states is overcomplete, the resolution of identity is not unique. We will be using the form:

$$\frac{2S+1}{4\pi}\int d\vec{\Omega}|\vec{\Omega}\rangle\langle\vec{\Omega}| = \frac{2S+1}{4\pi}\int_{-\pi}^{\pi}d\phi\int_0^{\pi}\sin\theta d\theta|\vec{\Omega}\rangle\langle\vec{\Omega}| = 1 \tag{1.78}$$

Proof: we use Eq. (1.76); the integral over ϕ is trivial, and we are left with:

$$\frac{2S+1}{4\pi}\int d\vec{\Omega}|\vec{\Omega}\rangle\langle\vec{\Omega}| = \frac{2S+1}{2}\int_0^{\pi}\sin\theta d\theta\sum_m\frac{(2S)!}{(S+m)!(S-m)!}\left[\frac{1+\cos\theta}{2}\right]^{S+m}\left[\frac{1-\cos\theta}{2}\right]^{S-m}|S,m\rangle\langle S,m|$$

We use the generating functional:

$$f(\lambda) = \int_0^{\pi}\sin\theta d\theta\sum_m\frac{(2S)!}{(S+m)!(S-m)!}\left[\frac{1+\cos\theta}{2}\right]^{S+m}\left[\frac{1-\cos\theta}{2}\right]^{S-m}\lambda^{S-m} = \int_{-1}^{1}du\left[\frac{1+\lambda+u(1-\lambda)}{2}\right]^{2S}$$

The integral is trivial, and we find

$$f(\lambda) = \frac{2}{2S+1}\frac{1-\lambda^{2S+1}}{1-\lambda} = \frac{2}{2S+1}\sum_{m=-S}^{S}\lambda^{S-m}$$

Since this is correct for any value of λ, it follows that for any m, that complicated integral equals $2/(2S+1)$, and so:

$$\frac{2S+1}{4\pi}\int d\vec{\Omega}|\vec{\Omega}\rangle\langle\vec{\Omega}| = \sum_{m=-S}^{S}|S,m\rangle\langle S,m| = 1$$

Another very useful identity, that can be proved similarly (assignment!) is:

$$\frac{(S+1)(2S+1)}{4\pi}\hbar\int d\vec{\Omega}\Omega_\alpha|\vec{\Omega}\rangle\langle\vec{\Omega}| = \hat{S}_\alpha, \qquad \alpha = 1,2,3. \tag{1.79}$$

We are finally ready to discuss spin path integrals. The steps will be very similar to the ones we went through in the previous sections.

1.8.3 Path integral

The amplitude of probability for the system to evolve from $|S,m_i\rangle$ at t_i to $|S,m_f\rangle$ at $t_f > t_i$ is:

$$\mathcal{G}(m_f,t_f;m_i,t_i) = \left(\frac{2S+1}{4\pi}\right)^2\int d\vec{\Omega}_i\int d\vec{\Omega}_f\langle S,m_f|\vec{\Omega}_i\rangle\mathcal{G}(\vec{\Omega}_f,t_f;\vec{\Omega}_i,t_i)\langle\vec{\Omega}_f|S,m_i\rangle$$

where

$$\mathcal{G}(\vec{\Omega}_f,t_f;\vec{\Omega}_i,t_i) = \Theta(t_f-t_i)\langle\vec{\Omega}_f|\mathbf{T}e^{-\frac{i}{\hbar}\int_{t_i}^{t_f}d\tau\hat{H}(\tau)}|\vec{\Omega}_i\rangle$$

which we need to calculate. We again divide the time interval into N parts of timelength $\epsilon = \Delta t/N$, and insert the resolution of identity $N-1$ times, and rename $\vec{\Omega}_i \equiv \vec{\Omega}_0$, $\vec{\Omega}_f \equiv \vec{\Omega}_N$, to obtain:

$$\mathcal{G}(\vec{\Omega}_f,t_f;\vec{\Omega}_i,t_i) = \lim_{N\to\infty}\left(\frac{2S+1}{4\pi}\right)^{N-1}\int d\vec{\Omega}_1\cdots\int d\vec{\Omega}_{N-1}\prod_{j=1}^{N}\langle\vec{\Omega}_j|\mathbf{T}e^{-\frac{i}{\hbar}\int_{t_{j-1}}^{t_j}d\tau\hat{H}(\tau)}|\vec{\Omega}_{j-1}\rangle$$

We define:

$$H[\vec{\Omega}(\tau)] = \frac{\langle\vec{\Omega}(\tau)|\hat{H}(\tau)|\vec{\Omega}(\tau-\epsilon)\rangle}{\langle\vec{\Omega}(\tau)|\vec{\Omega}(\tau-\epsilon)\rangle}$$

This is a quantity that can be computed once we are given the Hamiltonian $\hat{H}(t)$. As we did before, we calculate the matrix elements up to $\mathcal{O}(\epsilon^2)$:

$$\langle\vec{\Omega}_j|\mathbf{T}e^{-\frac{i}{\hbar}\int_{t_{j-1}}^{t_j}d\tau\hat{H}(\tau)}|\vec{\Omega}_{j-1}\rangle = \langle\vec{\Omega}_j|\vec{\Omega}_{j-1}\rangle e^{-\frac{i}{\hbar}\epsilon H[\vec{\Omega}(\tau_j)]} + \mathcal{O}(\epsilon^2)$$

The overlap is given by Eq. (1.77), and we again keep only terms up to ϵ in the expansion: $\theta(\tau-\epsilon) \approx \theta(\tau) - \epsilon\dot{\theta} + ...$, and similarly for the other angles. Collecting various powers of ϵ, we find that:

$$\left(\frac{1+\vec{\Omega}_j\cdot\vec{\Omega}_{j-1}}{2}\right)^S = 1 + \mathcal{O}(\epsilon^2)$$

$$\psi = -\epsilon\dot{\chi} - \epsilon\dot{\phi}\cos[\theta(\tau)] + \mathcal{O}(\epsilon^2)$$

and therefore:

$$\langle\vec{\Omega}_j|\vec{\Omega}_{j-1}\rangle = e^{iS\epsilon(\dot{\phi}\cos\theta(\tau)+\dot{\chi})} + \mathcal{O}(\epsilon^2)$$

such that:

$$\mathcal{G}(\vec{\Omega}_f,t_f;\vec{\Omega}_i,t_i) = \lim_{N\to\infty}\left(\frac{2S+1}{4\pi}\right)^{N-1}\int d\vec{\Omega}_1\cdots\int d\vec{\Omega}_{N-1}e^{iS\int_{t_i}^{t_f}d\tau\dot{\phi}(\tau)\cos\theta(\tau)-\frac{i}{\hbar}\int_{t_i}^{t_f}d\tau H[\vec{\Omega}(\tau)]} \tag{1.80}$$

which indeed has the expected form:

$$\mathcal{G}(\vec{\Omega}_f,t_f;\vec{\Omega}_i,t_i) = \sum_{\text{all paths}} e^{\frac{i}{\hbar}\int_{t_i}^{t_f}d\tau\mathcal{L}(\vec{\Omega},\dot{\vec{\Omega}},\tau)}$$

where

$$\mathcal{L}(\vec{\Omega},\dot{\vec{\Omega}},\tau) = \hbar S\dot{\phi}(\tau)\cos\theta(\tau) - H[\vec{\Omega}(\tau)] \tag{1.81}$$

Comments:

(1) we dropped the term $\int_{t_i}^{t_f}d\tau\dot{\chi}(\tau) = \chi(t_f) - \chi(t_i)$ from the exponent because it just gives a trivial phase shift. As I said, this is just a gauge transformation.

(2) the first term in the Lagrangian is purely quantum mechanical in nature, because it vanishes if $\hbar \to 0$. The corresponding action,

$$\omega[\vec{\Omega}] = \int_{t_i}^{t_f}d\tau\dot{\phi}(\tau)\cos\theta(\tau)$$

is called **the Berry phase**. We will later discuss an alternative way of writing this term, that makes its meaning more transparent.

(3) both here and in all the previous path integrals we considered: when we make approximations of the type $x(\tau+\epsilon) = x(\tau) + \epsilon\dot{x} + ...$ for any quantity x, we implicitly assume that the dominant contribution to $\mathcal{G}$ is from paths that are smooth, i.e. with $\dot{x} < \infty$. Generally, this procedure is unjustified; by ignoring discontinuous paths, we loose information about the ordering of the operators in the quantum Hamiltonian (classically $xp_x = p_x x$, but this is not true in quantum mechanics. If such ambiguous terms appear, one must be more careful). The point is that if you ever need to work with path integrals in some representation that was not previously considered by others, you need to

validate the final expression you obtain by doing such expansions – for instance, by checking against perturbation theory results in the limit when some term in the Hamiltonian becomes small.

(4) for the Hamiltonian of Eq. (1.68), we have:

$$H[\vec{\Omega}(\tau)] = -\vec{h}(\tau)\cdot\langle\vec{\Omega}(\tau)|\hat{\vec{S}}|\vec{\Omega}(\tau)\rangle + \mathcal{O}(\epsilon) = \hbar S\left[-\vec{h}(\tau)\cdot\vec{\Omega}(\tau)\right] + \ldots$$

This is a very intuitive form (which you should check!). Then, the action is:

$$\frac{1}{\hbar S}S_{action} = \int_{t_i}^{t_f} d\tau\left[\dot{\phi}(\tau)\cos\theta(\tau) + \vec{h}(\tau)\cdot\vec{\Omega}(\tau)\right]$$

What are the "classical" equations of motion (if we take $\hbar \to 0$, but $S \to \infty$)? Requesting that $\delta S_{action} = 0$ we find the equation of motion:

$$\vec{\Omega}\times\dot{\vec{\Omega}} = -\vec{h}(\tau) \to \dot{\vec{\Omega}}_{cl} = \vec{\Omega}_{cl}\times\vec{h}(\tau)$$

where to obtain the second equality, we use $\vec{\Omega}\cdot\vec{\Omega} = 1 \to \vec{\Omega}\cdot\dot{\vec{\Omega}} = 0$. This equation describes the expected precession of the spin about the magnetic field. The equation is identical to the one we obtain in quantum mechanics:

$$i\hbar\frac{d}{dt}\hat{S}_\alpha(t) = [\hat{S}_\alpha(t), \hat{H}] = i\hbar\epsilon_{\alpha\beta\gamma}\hat{S}_\gamma h_\beta \to \frac{d}{dt}\hat{\vec{S}} = \hat{\vec{S}}\times\vec{h}(t)$$

Taking the expectation value of this would lead to the same "classical" equation. For more general Hamiltonians, the "classical" equation is:

$$\dot{\vec{\Omega}}_{cl} = -\vec{\Omega}_{cl}\times\left.\frac{\partial H[\vec{\Omega}]}{\partial\vec{\Omega}}\right|_{\vec{\Omega}=\vec{\Omega}_{cl}}$$

which is the direct analog of the so-called Landau-Lifshitz equation.

Remember that the standard way of computing a path integral was to expand about the classical trajectory. One very peculiar thing about the "classical" equation, here, is that it has only a first order time derivative, meaning that we need only one initial condition $\vec{\Omega}(t_i) = \vec{\Omega}_i$ to fully determine the solution. Also, the dependence on $\cos(\theta)$ in the Berry phase suggests that the expansion may be rather messy.

To appreciate the usefulness of this expression, one must actually investigate systems of interacting spins. For instance, we can see that half-integer and integer spin systems may behaved very differently. Imagine that we consider the contribution to $\mathcal{G}$ of pairs of paths, for which the Berry phases differ by exactly 2π. Then, for an integer-spin, $e^{iS2\pi} = 1$ and the two paths interfere constructively. On the other hand, for a half-integer spin $e^{iS2\pi} = -1$ and we have destructive interference. One such difference which can be traced back to Berry phases (project?) is that 1D AFM chains are gapless for half-integer spins whereas they are gapped for integer spins. For a gapped system, one needs to pay a certain, finite amount of energy to create an excitation, whereas in a gapless system there are excitations which cost zero (infinitesimally small) energy.

Two more interesting facts about the Berry phase:

(a) using $\dot{\vec{\Omega}} = \dot{\theta}\vec{e}_\theta +]sin\theta\dot{\phi}\vec{e}_\phi$ and defining

$$\vec{A}(\vec{\Omega}) = \frac{\cos\theta}{\sin\theta}\vec{e}_\phi$$

we can rewrite the Berry phase as:

$$S\omega[\vec{\Omega}] = S\int_{t_i}^{t_f} d\tau \dot{\vec{\Omega}} \cdot \vec{A}$$

This term describes an electric charge of magnitude S which is constrained to move on the surface of the unit sphere ($\vec{\Omega}$ describes its location) in the magnetic field of a monopole located at the origin ($\vec{A}$ is its vector potential).

(b) the Berry phase has an interesting geometrical interpretation, since:

$$\omega[\vec{\Omega}] = \int_{t_i}^{t_f} d\tau \dot{\phi}(\tau)\cos\theta(\tau) = \int_{\phi_i}^{\phi_f} d\phi \cos\theta(\phi)$$

This shows that this phase is geometric in nature, depending only on the shape of the trajectory described by $\vec{\Omega}$, but not on its explicit time dependence. In fact, for a closed path on the surface of the sphere, the Berry phase $\omega[\vec{\Omega}]$ just measures the area "enclosed" by the trajectory, which is the same as the solid angle subextended by the closed curve (the sphere has a unit radius). The reason I use quotation marks is because the enclosed area is only defined up to 4π, since it could be the area on either side of the curve, and the two add up to 4π. Things are well defined provided that this 4π uncertainty plays no role in the results, which implies that $e^{iS4\pi} = 1$, i.e. S must be an integer or a half-integer.

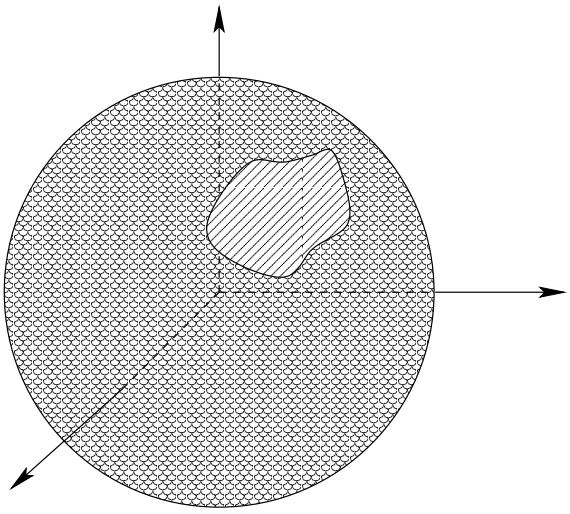

Figure 1.16: Geometrical interpretation of the Berry phase. For a closed path, it equals the area "enclosed" by the path, which is defined only modulo 4π.