The Path Integral approach to Quantum Mechanics
Lecture Notes for Quantum Mechanics IV

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Chapter 1

The path integral formalism

1.1 Introducing the path integrals

1.1.1 The double slit experiment

One of the important experiments that show the fundamental difference between Quantum and Classical Mechanics is the double slit experiment. It is interesting with respect to the path integral formalism because it leads to a conceptual motivation for introducing it.

Consider a source S of approximately monoenergetic particles, electrons for instance, placed at position A. The flux of electrons is measured on a screen C facing the source. Imagine now placing a third screen in between the others, with two slits on it, which can be opened or closed (see figure 1.1). When the first slit is open and the second closed we measure a flux F_1, when the first slit is closed and the second open we measure a flux F_2 and when both slits are open we measure a flux F.
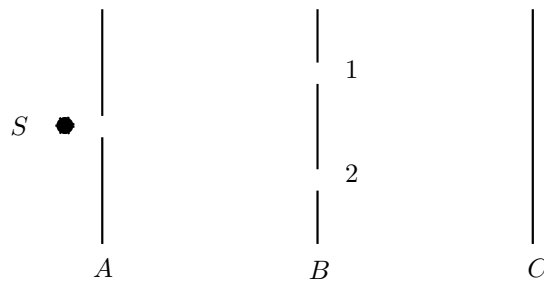
Figure 1.1: The double slit experiment: an electron source is located somewhere on A, and a detector is located on the screen C. A screen B with two slits 1 and 2 that can be open or closed is placed in between, so that the electrons have to pass through 1 or 2 to go from A to C. We measure the electron flux on the screen C.

In classical physics, the fluxes at C in the three cases are expected to satisfy the relation $F = F_1 + F_2$. In reality, one finds in general $F = F_1 + F_2 + F_{int}$, and the structure of F_{int} precisely corresponds to the interference between two

waves passing respectively through 1 and 2:

$$F = |\Phi_1 + \Phi_2|^2 = \underbrace{|\Phi_1|^2}_{F_1} + \underbrace{|\Phi_2|^2}_{F_2} + \underbrace{2\,\mathrm{Re}\left(\Phi_1^*\Phi_2\right)}_{F_{int}} \qquad (1.1)$$

How can we interpret this result? What is the electron?

More precisely: Does the wave behaviour imply that the electron is a delocalized object? That the electron is passing through both slits?

Actually not. When detected, the electron is point-like, and more remarkably, if we try to detect where it went through, we find that it either goes through 1 or 2 (this is done by setting detectors at 1 and 2 and considering a very weak flux, in order to make the probability of coinciding detections at 1 and 2 arbitrarily small).

According to the Copenhagen interpretation, F should be interpreted as a probability density. In practice this means: compute the amplitude Φ as if dealing with waves, and interpret the intensity $|\Phi|^2$ as a probability density for a point-like particle position.

How is the particle/wave duality not contradictory? The answer is in the indetermination principle. In the case at hand: when we try to detect which alternative route the electron took, we also destroy interference. Thus, another formulation of the indetermination principle is: Any determination of the alternative taken by a process capable of following more than one alternative destroys the interference between the alternatives.

Resuming:

- What adds up is the amplitude Φ and not the probability density itself.

- The difference between classical and quantum composition of probabilities is given by the interference between classically distinct trajectories.

In the standard approach to Quantum Mechanics, the probability amplitude is determined by the Schrödinger equation. The "Schrödinger" viewpoint somehow emphasizes the wave properties of the particles (electrons, photons, ...). On the other hand, we know that particles, while they are described by "a probability wave", are indeed point-like discrete entities. As an example, in the double slit experiment, one can measure where the electron went through (at the price of destroying quantum interference).

This course will present an alternative, but fully equivalent, method to compute the probability amplitude. In this method, the role of the trajectory of a point-like particle will be formally "resurrected", but in a way which is compatible with the indetermination principle. This is the path integral approach to Quantum Mechanics. How can one illustrate the basic idea underlying this approach?

1.1.2   An intuitive approach to the path integral formalism

In the double slit experiment, we get two interfering alternatives for the path of electrons from A to C. The idea behind the path integral approach to Quantum Mechanics is to take the implications of the double slit experiment to its extreme consequences. One can imagine adding extra screens and drilling more and more

holes through them, generalizing the result of the double slit experiment by the superposition principle. This is the procedure illustrated by Feynman in his book "Quantum Mechanics and Path Integrals".

Schematically:

- With two slits: we know that $\Phi = \Phi_1 + \Phi_2$

- If we open a third slit, the superposition principle still applies: $\Phi = \Phi_1 + \Phi_2 + \Phi_3$

- Imagine then adding an intermediate screen D with N holes at positions $x_D^1, x_D^2, \ldots, x_D^N$ (see figure 1.2). The possible trajectories are now labelled by x_D^i and $\alpha = 1, 2, 3$, that is by the slit they went through at D and by the slit they went through at B.
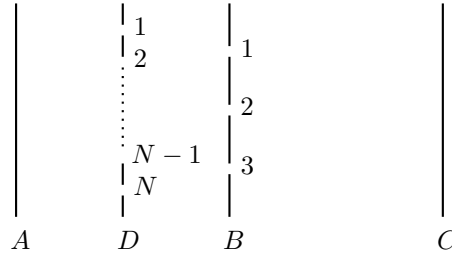
Figure 1.2: The multi-slit experiment: We have a screen with N slits and a screen with three slits placed between the source and the detector.

Applying the superposition principle:

$$\Phi = \sum_{i=1}^{N} \sum_{\alpha=1,2,3} \Phi\left(x_D^i, \alpha\right)$$

Nothing stops us from taking the <u>ideal</u> limit where $N \to \infty$ and the holes fill all of D. The sum $\sum_i$ becomes now an integral over x_D.

$$\Phi = \sum_{\alpha=1,2,3} \int dx_D \, \Phi\left(x_D, \alpha\right)$$

D is then a purely fictious device! We can go on and further refine our trajectories by adding more and more fictious screens $D_1, D_2, \ldots, D_M$

$$\Phi = \sum_{\alpha=1,2,3} \int dx_{D_1} dx_{D_2} \cdots dx_{D_M} \, \Phi\left(x_{D_1}, x_{D_2}, \ldots, x_{D_M}; \alpha\right)$$

In the limit in which D_i, D_{i+1} become infinitesimally close, we have specified all possible paths $x(y)$ (see figure 1.3 for a schematic representation, where the screen B has been dropped in order to consider the simpler case of propagation in empty space).
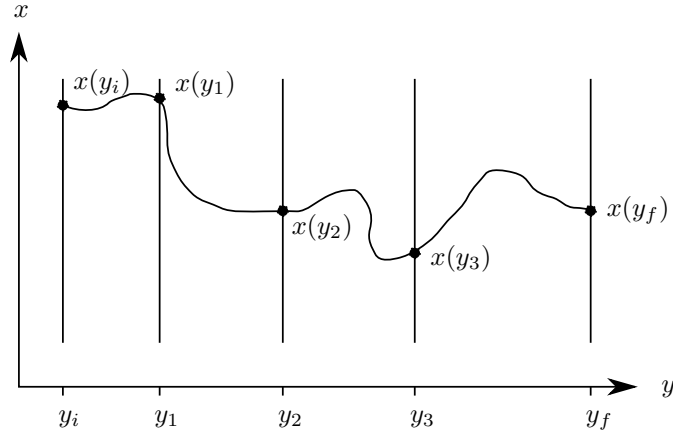
Figure 1.3: The paths from (x_i, y_i) to (x_f, y_f) are labelled with the functions $x(y)$ that satisfy $x(y_i) = x_i$ and $x(y_f) = x_f$.

In fact, to be more precise, also the way the paths are covered through time is expected to matter $(t \to (x(y), y(t)))$. We then arrive at a formal representation of the probability amplitude as a sum over all possible trajectories:

$$\Phi = \sum_{\substack{\text{All} \\ \text{trajectories} \\ \{x(t), y(t)\}}} \Phi(\{x\}) \tag{1.2}$$

How is this formula made sense of? How is it normalized?

1.1.3   The path integral formulation

Based on the previous section, we will start anew to formulate quantum mechanics. We have two guidelines:

1. We want to describe the motion from position x_i at time t_i to position x_f at time t_f with a quantum probability amplitude $K(x_f, t_f; x_i, t_i)$ given by

$$K(x_f, t_f; x_i, t_i) = \sum_{\substack{\text{All} \\ \text{trajectories}}} \Phi(\{\gamma\})$$

   where $\{\gamma\}$ is the set of all trajectories satisfying $x(t_i) = x_i$, $x(t_f) = x_f$.

2. We want classical trajectories to describe the motion in the formal limit $\hbar \to 0$. In other words, we want classical physics to be resurrected in the $\hbar \to 0$ limit.

Remarks:

- $\hbar$ has the dimensionality [Energy] $\times$ [Time]. That is also the dimensionality of the action S which describes the classical trajectories via the principle of least action.

- One can associate a value of $S[\gamma]$ to each trajectory. The classical trajectories are given by the stationary points of $S[\gamma]$ ($\delta S[\gamma] = 0$).

It is thus natural to guess: $\Phi[\gamma] = f(S[\gamma]/\hbar)$, with f such that the classical trajectory is selected in the formal limit $\hbar \to 0$. The specific choice

$$\Phi[\gamma] = e^{i\frac{S[\gamma]}{\hbar}} \tag{1.3}$$

implying

$$K(x_f, t_f; x_i, t_i) = \sum_{\{\gamma\}} e^{i\frac{S[\gamma]}{\hbar}} \tag{1.4}$$

seems promising for two reasons:

1. The guideline (2.) is heuristically seen to hold. In a macroscopic, classical, situation the gradient $\delta S/\delta\gamma$ is for most trajectories much greater than $\hbar$. Around such trajectories the phase $e^{iS/\hbar}$ oscillates extremely rapidly and the sum over neighbouring trajectories will tend to cancel. [1] (see figure 1.4).
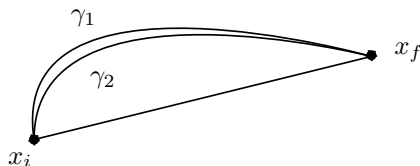
Figure 1.4: The contributions from the two neighbouring trajectories γ_1 and γ_2 will tend to cancel if their action is big.
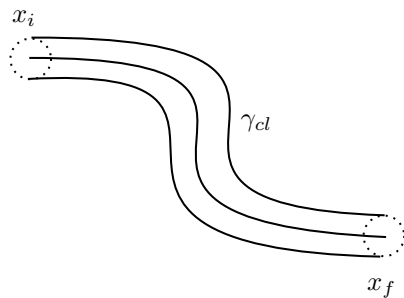
Figure 1.5: The contributions from the neighbouring trajectories of the classical trajectory will dominate.

On the other hand, at a classical trajectory γ_{cl} the action $S[\gamma]$ is stationary. Therefore in the neighbourhood of γ_{cl}, S varies very little, so that all trajectories in a tube centered around γ_{cl} add up coherently (see figure 1.5) in the sum over trajectories. More precisely: the tube of trajectories

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[1] By analogy, think of the integral $\int_{-\infty}^{+\infty} dx e^{if(x)}$ where $f(x) \equiv ax$ plays the role of $S/\hbar$: the integral vanishes whenever the derivative of the exponent $f' = a$ is non-zero

in question consists of those for which $|S - S_{cl}| \leq \hbar$ and defines the extent to which the classical trajectory is well defined. We cannot expect to define our classical action to better than $\sim \hbar$. However, in normal macroscopic situations $S_{cl} \gg \hbar$. In the exact limit $\hbar \to 0$, this effect becomes dramatic and only the classical trajectory survives.

Once again, a simple one dimensional analogy is provided by the integral $\int_{-\infty}^{+\infty} dx e^{ix^2/h}$, which is dominated by the region $x^2 \lesssim h$ around the stationary point $x = 0$.

2. Eq. (1.3) leads to a crucial composition property. Indeed the action for a path γ_{12} obtained by joining two subsequent paths γ_1 and γ_2, like in fig. 1.6, satisfies the simple additive relation $S[\gamma_{12}] = S[\gamma_1] + S[\gamma_2]$. Thanks to eq. (1.3) the additivity of S translates into a factorization property for the amplitude: $\Phi[\gamma_{12}] = \Phi[\gamma_1]\Phi[\gamma_2]$ which in turn leads to a composition property of K, which we shall now prove.

Consider indeed the amplitudes for three consecutive times $t_i < t_{int} < t_f$. The amplitude $K(x_f, t_f; x_i, t_i)$ should be obtainable by evolving in two steps: first from t_i to t_{int} (by $K(y, t_{int}; x_i, t_i)$ for any y), and second from t_{int} to t_f (by $K(x_f, t_f; y, t_{int})$. Now, obviously each path with $x(t_i) = x_i$ and $x(t_f) = x_f$ can be obtained by joining two paths $\gamma_1(y = x(t_{int}))$ from t_i to t_{int} and $\gamma_2(y = x(t_{int}))$ from t_{int} to t_f (see figure 1.6).
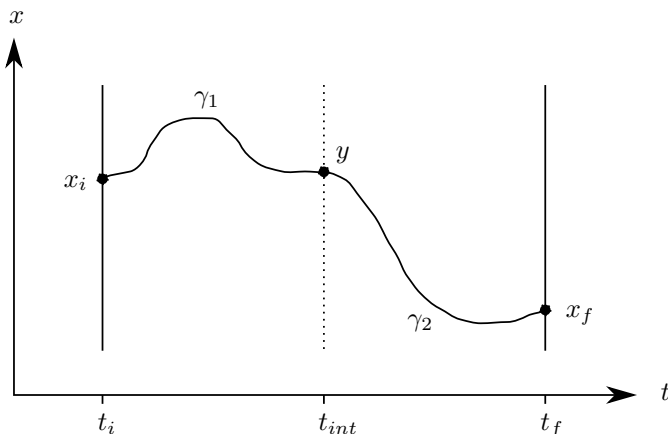
Figure 1.6: The path from (x_i, t_i) to (x_f, t_f) can be obtained by summing the paths γ_1 from (x_i, t_i) to (y, t_{int}) with γ_2 from (y, t_{int}) to (x_f, t_f).

Thanks to eq. (1.3) we can then write:

$$\int dy K(x_f, t_f; y, t_{int}) K(y, t_{int}; x_i, t_i)$$

$$= \sum_{\gamma_1, \gamma_2} \int dy \, e^{\frac{i}{\hbar}(S[\gamma_1(y)] + S[\gamma_2(y)])}$$

$$= \sum_{\gamma(y) = \gamma_2(y) \circ \gamma_1(y)} \int dy \, e^{\frac{i}{\hbar} S[\gamma(y)]}$$

$$= K(x_f, t_f; x_i, t_i) \,. \tag{1.5}$$

Notice that the above composition rule is satisfied in Quantum Mechanics as easily seen in the usual formalism. It is the quantum analogue of the classical composition of probabilities

$$P_{1 \to 2} = \sum_\alpha P_{1 \to \alpha} P_{\alpha \to 2} \,. \tag{1.6}$$

In quantum mechanics what is composed is not probability P itself but the amplitude K which is related to probability by $P = |K|^2$.

It is instructive to appreciate what would go wrong if we modified the choice in eq. (1.3). For instance the alternative choice $\Phi = e^{-S[\gamma]/\hbar}$ satisfies the composition property but does not in general select the classical trajectories for $\hbar \to 0$. This alternative choice would select the minima of S but the classical trajectories represent in general only saddle points of S in function space. Another alternative $\Phi = e^{i(S[\gamma]/\hbar)^2}$, would perhaps work out in selecting the classical trajectories for $\hbar \to 0$, but it would not even closely reproduce the composition property we know works in Quantum Mechanics. (More badly: this particular choice, if S were to represent the action for a system of two particles, would imply that the amplitudes for each individual particle do not factorize even in the limit in which they are very far apart and non-interacting!).

One interesting aspect of quantization is that a fundamental unit of action ($\hbar$) is introduced. In classical physics the overall value of the action in unphysical: if

$$S(q, \dot{q}) \quad \to \quad S_\lambda \equiv \lambda S(q, \dot{q}) \tag{1.7}$$

the only effect is to multiply all the equations of motion by λ, so that the solutions remain the same (the stationary points of S and S_λ coincide).

Quantum Mechanics sets a natural unit of measure for S. Depending on the size of S, the system will behave differently:

- large $S \to$ classical regime

- small $S \to$ quantum regime

In the large S limit, we expect the trajectories close to γ_{cl} to dominate K (semiclassical limit). We expect to have: $K(x_f; x_i) \sim$ (smooth function) $\cdot e^{i \frac{S_{cl}}{\hbar}}$.

In the $S \sim \hbar$ limit, all trajectories are comparably important: we must sum them up in a consistent way; this is not an easy mathematical task.

Due to the mathematical difficulty, rather than going on with Feynman's construction and show that it leads to the same results of Schrödinger equation, we will follow the opposite route which is easier: we will derive the path integral formula from Schrödinger's operator approach.

1.1.4   From the Schröedinger approach to the path integral

Consider the transition amplitude:

$$K(x_f, t_f; x_i, t_i) \equiv \langle x_f | e^{-\frac{iH(t_f - t_i)}{\hbar}} | x_i \rangle = \langle x_f | e^{-\frac{iHt}{\hbar}} | x_i \rangle \qquad (1.8)$$

where we used time translation invariance to set: $t_i = 0$, $t_f - t_i = t$.

To write it in the form of a path integral, we divide t into N infinitesimal steps and consider the amplitude for each infinitesimal step (see figure 1.7). We label the intermediate times $t_k = k\epsilon$ by the integer $k = 0, \dots, N$. Notice that $t_0 = 0$ and $t_N = t$.

Figure 1.7: The interval between 0 and t is divided into N steps.

We can use the completeness relation $\int |x\rangle \langle x| \, dx = 1$ at each step $n\epsilon$:

$$\langle x_f | e^{-\frac{iHt}{\hbar}} | x_i \rangle = \int \prod_{k=1}^{N-1} dx_k \, \langle x_f | e^{-\frac{iH\epsilon}{\hbar}} | x_{N-1} \rangle \langle x_{N-1} | e^{-\frac{iH\epsilon}{\hbar}} | x_{N-2} \rangle \cdots$$
$$\langle x_2 | e^{-\frac{iH\epsilon}{\hbar}} | x_1 \rangle \langle x_1 | e^{-\frac{iH\epsilon}{\hbar}} | x_i \rangle \quad (1.9)$$

Consider the quantity: $\langle x' | e^{-iH\epsilon/\hbar} | x \rangle$. Using $\int |p\rangle \langle p| \, dp = 1$:

$$\langle x' | e^{-\frac{iH\epsilon}{\hbar}} | x \rangle = \int dp \, \langle x'|p\rangle \langle p | e^{-\frac{iH\epsilon}{\hbar}} | x \rangle \qquad (1.10)$$

If we stick to the simple case $H = \frac{\hat{p}^2}{2m} + V(\hat{x})$, we can write:

$$\langle p | e^{-i\frac{\epsilon}{\hbar}\left[\frac{\hat{p}^2}{2m} + V(\hat{x})\right]} | x \rangle = e^{-i\frac{\epsilon}{\hbar}\left[\frac{p^2}{2m} + V(x)\right]} \langle p|x \rangle + \mathcal{O}\left(\epsilon^2\right) \qquad (1.11)$$

where the $O(\epsilon^2)$ terms arise from the non-vanishing commutator between $\hat{p}^2/(2m)$ and $V(\hat{x})$. We will now assume, which seems fully reasonable, that in the limit $\epsilon \to 0$ these higher orer terms can be neglected. Later on we shall come back on this issue and better motivate our neglect of these terms.

We then get:

$$\langle x' | e^{-\frac{iH\epsilon}{\hbar}} | x \rangle \simeq \int dp \left[e^{-i\frac{\epsilon}{\hbar}\left[\frac{p^2}{2m} + V(x)\right]} \cdot \frac{e^{\frac{i}{\hbar}p(x'-x)}}{2\pi\hbar} \right] \qquad (1.12)$$

We can define: $\frac{x'-x}{\epsilon} \equiv \dot{x}$:

$$\langle x' | e^{-\frac{iH\epsilon}{\hbar}} | x \rangle \simeq \int \frac{dp}{2\pi\hbar} e^{-i\frac{\epsilon}{\hbar}\left[\frac{p^2}{2m} + V(x) - p\dot{x}\right]} \qquad (1.13)$$

By performing the change of variables $\bar{p} \equiv p - m\dot{x}$ the integral reduces to simple gaussian integral for the variable $\bar{p}$:

$$\langle x' | e^{-\frac{iH\epsilon}{\hbar}} | x \rangle \simeq \int \frac{d\bar{p}}{2\pi\hbar} e^{-i\frac{\epsilon}{\hbar}\left[\frac{\bar{p}^2}{2m} + V(x) - \frac{m\dot{x}^2}{2}\right]} \tag{1.14}$$

$$= \underbrace{\sqrt{\frac{m}{2\pi i \hbar \epsilon}}}_{\frac{1}{A}} e^{i\frac{\epsilon}{\hbar}\left[\frac{1}{2}m\dot{x}^2 - V(x)\right]} = \frac{1}{A} e^{i\mathcal{L}(x,\dot{x})\frac{\epsilon}{\hbar}} \tag{1.15}$$

At leading order in ϵ we can further identify $\mathcal{L}(x,\dot{x})\epsilon$ with the action $S(x',x) = \int_0^\epsilon \mathcal{L}(x,\dot{x})dt$. By considering all the intervals we thus finally get:

$$\langle x_f | e^{-\frac{iHt}{\hbar}} | x_i \rangle = \lim_{\epsilon \to 0} \int \prod_{k=1}^{N-1} dx_k \frac{1}{A^N} e^{\frac{i}{\hbar} \sum_{l=0}^{N-1} S(x_{l+1}, x_l)}$$

$$= \lim_{\epsilon \to 0} \frac{1}{A} \underbrace{\int \prod_{k=1}^{N-1} \frac{dx_k}{A}}_{\int D\gamma} e^{i\frac{S(x_f, x_i)}{\hbar}} \tag{1.16}$$

where $\int D\gamma$ should be taken as a definition of the functional measure over the space of the trajectories. We thus have got a path integral formula for the transition amplitude:

$$K(x_f, t; x_i, 0) = \int \mathscr{D}[x(t)] e^{i\frac{S_{cl}(x,\dot{x})}{\hbar}} \tag{1.17}$$

We see that we (actually somebody else before us!) had guessed well the form of the transition amplitude. The path integral approach to QM was developed by Richard Feyman in his PhD Thesis in the mid 40's, following a hint from an earlier paper by Dirac. Dirac's motivation was apparently to formulate QM starting from the lagrangian rather than from the hamiltonian formulation of classical mechanics.

Let us now come back to the neglected terms in eq. (1.11). To simplify the notation let us denote the kinetic operator as $T = -i\frac{p^2}{2m\hbar}$ and the potential $U = -iV/\hbar$; we can then write

$$\langle p | e^{\epsilon(T+U)} | x \rangle = \langle p | e^{\epsilon T} e^{-\epsilon T} e^{\epsilon(T+U)} e^{-\epsilon U} e^{\epsilon U} | x \rangle = \langle p | e^{\epsilon T} e^{-\epsilon^2 C} e^{\epsilon U} | x \rangle \tag{1.18}$$

$$= e^{-i\frac{\epsilon}{\hbar}\left[\frac{p^2}{2m} + V(x)\right]} \langle p | e^{-\epsilon^2 C} | x \rangle \tag{1.19}$$

where C is given, by using the Campbell-Baker-Haussdorf formula twice, as a series of commutators between T and U

$$C = \frac{1}{2}[T, U] + \frac{\epsilon}{6} \left\{[T, [T, U]] + [U, [U, T]]\right\} + \dots \tag{1.20}$$

By iterating the basic commutation relation $[\hat{p}, V(\hat{x})]] = -iV'(\hat{x})$ and expanding the exponent in a series one can then write

$$\langle p | e^{-\epsilon^2 C} | x \rangle = 1 + \epsilon \sum_{n=0}^{n=\infty} \sum_{r=1}^{r=n} \sum_{s=0}^{s=r} \epsilon^n p^{r-s} P_{n,s,r}(x) \tag{1.21}$$

where $P_{n,s,r}(x)$ is a homogenous polynomial of degree $n + 1 - r$ in V and its derivatives, with each term involving exactly $r + s$ derivatives. For instance $P_{1,0,1}(x) = V'(x)$. We can now test our result under some simple assumption. For instance, if the derivatives of V are all bounded, the only potential problem to concentrate on in the $\epsilon \to 0$ limit is represented by the powers of p. This is because the leading contribution to the p integral in eq. (1.15) comes from the region $p \sim 1/\sqrt{\epsilon}$, showing that p diverges in the small ϵ limit. By using $p \sim 1/\sqrt{\epsilon}$ the right hand side of eq. (1.21) is $\sim 1 + O(\epsilon^{3/2})$ so that, even taking into account that there are $N \sim 1/\epsilon$ such terms (one for each step), the final result is still convergent to 1

$$\lim_{\epsilon \to 0} \left(1 + a\epsilon^{\frac{3}{2}} \right)^{\frac{1}{\epsilon}} = 1 \, . \tag{1.22}$$

Before proceeding with technical developments, it is worth assessing the rôle of the path integral (P.I.) in quantum mechanics. As it was hopefully highlighted in the discussion above, the path integral formulation is conceptually advantageous over the standard operatorial formulation of Quantum Mechanics, in that the "good old" particle trajectories retain some rôle. The P.I. is however technically more involved. When working on simple quantum systems like the hydrogen atom, no technical profit is really given by path integrals. Nonetheless, after overcoming a few technical difficulties, the path integral offers a much more direct viewpoint on the semiclassical limit. Similarly, for issues involving topology like the origin of Bose and Fermi statistics, the Aharonov-Bohm effect, charge quantization in the presence of a magnetic monopole, etc. . . path integrals offer a much better viewpoint. Finally, for advanced issues like the quantization of gauge theories and for effects like instantons in quantum field theory it would be hard to think how to proceed without path integrals!...But that is for another course.

1.2   The properties of the path integrals

1.2.1   Path integrals and state evolution

To get an estimate of the dependence of the amplitude $K(x_f, t_f; x_i, t_i)$ on its arguments, let us first look at the properties of the solutions to the classical equations of motion with boundary conditions $x_c(t_i) = x_i$, $x_c(t_f) = x_f$.

Let us compute $\partial_{t_f} S_{cl}$. Where S_{cl} is defined

$$S_{cl} \equiv S[x_c] = \int_{t_i}^{t_f} \mathcal{L}(x_c, \dot{x}_c) dt \tag{1.23}$$

with x_c a solution, satisfying the Euler-Lagrange equation:

$$\left[\partial_t \frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x} \right]_{x=x_c} = 0 \, . \tag{1.24}$$

We can think of x_c as a function

$$x_c \equiv f(x_i, x_f, t_i, t_f, t)$$

such that

$$f(x_i, x_f, t_i, t_f, t = t_i) \equiv x_i = const$$

$$f(x_i, x_f, t_i, t_f, t = t_f) \equiv x_f = const$$

Differentiating the last relation we deduce:

$$\left[\partial_{t_f} x_c + \partial_t x_c \right]_{t=t_f} = 0$$

$$\implies \left. \partial_{t_f} x_c \right|_{t=t_f} = -\left. \dot{x}_c \right|_{t=t_f} \tag{1.25}$$

Similarly, differentiating the relation at $t = t_i$ we obtain

$$\left. \partial_{t_f} x_c \right|_{t=t_i} = 0 \tag{1.26}$$

And the following properties are straightforward:

$$\left. \partial_{x_f} x_c \right|_{t=t_f} = 1 \tag{1.27}$$

$$\left. \partial_{x_f} x_c \right|_{t=t_i} = 0 \tag{1.28}$$

Using these properties, we can now compute:

$$\partial_{t_f} S = \left. \mathcal{L}(x, \dot{x}) \right|_{t=t_f} + \int_{t_i}^{t_f} dt \left[\frac{\partial \mathcal{L}}{\partial x} \partial_{t_f} x + \frac{\partial \mathcal{L}}{\partial \dot{x}} \partial_{t_f} \dot{x} \right]$$

$$= \left. \mathcal{L}(x, \dot{x}) \right|_{t=t_f} + \int_{t_i}^{t_f} dt \left[\partial_t \left(\frac{\partial \mathcal{L}}{\partial \dot{x}} \partial_{t_f} x \right) \right] - \int_{t_i}^{t_f} dt \left(\partial_t \frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x} \right) \partial_{t_f} x \tag{1.29}$$

All this evaluated at $x = x_c$ gives:

$$\partial_{t_f} S_{cl} = \left. \mathcal{L}(x_c, \dot{x}_c) \right|_{t=t_f} + \left(\left. \frac{\partial \mathcal{L}}{\partial \dot{x}} \right|_{x=x_c} \partial_{t_f} x_c \right) \Bigg|_{t=t_i}^{t=t_f}$$

$$= \left(\mathcal{L}(x_c, \dot{x}_c) - \left. \frac{\partial \mathcal{L}}{\partial \dot{x}} \right|_{x=x_c} \dot{x}_c \right) \Bigg|_{t=t_f} = -E \tag{1.30}$$

We recognize here the definition of the hamiltonian of the system, evaluated at $x = x_c$ and $t = t_f$.

We can also compute:

$$\partial_{x_f} S = \int_{t_i}^{t_f} dt \left[\partial_t \left(\frac{\partial \mathcal{L}}{\partial \dot{x}} \partial_{x_f} x \right) \right] - \int_{t_i}^{t_f} dt \left(\partial_t \frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x} \right) \partial_{x_f} x \tag{1.31}$$

Evaluated at $x = x_c$, this gives:

$$\partial_{x_f} S_{cl}(x_c) = \left(\left. \frac{\partial \mathcal{L}}{\partial \dot{x}} \right|_{x=x_c} \partial_{x_f} x_c \right) \Bigg|_{t=t_i}^{t=t_f} = \left. \frac{\partial \mathcal{L}}{\partial \dot{x}} \right|_{x=x_c, t=t_f} = P \tag{1.32}$$

We recognize here the definition of the momentum of the system, evaluated at $x = x_c$ and $t = t_f$.

At this point, we can compare these results with those of the path integral computation in the limit $\hbar \to 0$.

$$K(x_f, t_f; x_i, t_i) = \int \mathscr{D}[x(t)] e^{i\frac{S}{\hbar}} \tag{1.33}$$

In the limit $\hbar$ we expect the path integral to be dominated by the classical trajectory and thus to take the form (and we shall technically demostrate this expectation later on)

$$K(x_f, t_f; x_i, t_i) = \underbrace{F(x_f, t_f, x_i, t_i)}_{\text{smooth function}} e^{i\frac{S_{cl}}{\hbar}} \tag{1.34}$$

where F is a smooth function in the $\hbar \to 0$ limit. We then have:

$$\partial_{t,x} e^{i\frac{S_{cl}}{\hbar}} \sim \frac{1}{\hbar} \qquad\qquad \text{large} \tag{1.35}$$

$$\partial_{t,x} F \sim \mathcal{O}(1) \qquad\qquad \text{comparatively negligible} \tag{1.36}$$

so that we obtain

$$-i\hbar \partial_{x_f} K = \partial_{x_f} S_{cl} \cdot K + \mathcal{O}(\hbar) = P_{cl} K + \mathcal{O}(\hbar) \tag{1.37}$$

$$i\hbar \partial_{t_f} K = -\partial_{t_f} S_{cl} \cdot K + \mathcal{O}(\hbar) = E_{cl} K + \mathcal{O}(\hbar) \tag{1.38}$$

Momentum and energy, when going to the path integral description of particle propagation, become associated to respectively the wave number $(\sim (i\partial_x \ln K)^{-1})$ and oscillation frequency $(\sim (i\partial_t \ln K))$.

The last two equations make contact with usual quantum mechanical relations, if we interpret K has the wave function and $-i\hbar\partial_x$ and $i\hbar\partial_t$ as respectively the momentum and energy operators

$$-i\hbar \partial_x K \sim P \cdot K \tag{1.39}$$

$$i\hbar \partial_t K \sim E \cdot K \tag{1.40}$$

The function $K(x', t'; x, t) = \langle x' | e^{-\frac{iH(t'-t)}{\hbar}} | x \rangle$ is also known as the propagator, as it describes the probability amplitude for propagating a particle from x to x' in a time $t' - t$.

From the point of view of the Schrödinger picture, $K(x', t; x, 0)$ represents the wave function at time t for a particle that was in the state $|x\rangle$ at time 0:

$$\psi(t, x) \equiv \langle x | e^{-\frac{iHt}{\hbar}} | \psi_0 \rangle \equiv \langle x | \psi(t) \rangle \tag{1.41}$$

By the superposition principle, K can then be used to write the most general solution. Indeed:

1. $K(x', t'; x, t)$ solves the Schrödinger equation for t', x' as variables:

$$i\hbar \partial_{t'} K = \int dx'' H(x', x'') K(x'', t'; x, t) \tag{1.42}$$

where $H(x', x'') = \langle x' | H | x'' \rangle$.

2.

$$\lim_{t' \to t} K(x', t'; x, t) = \langle x' | x \rangle = \delta(x' - x)$$

Thus, given $\Psi_0(x)$ the wave function at time t_0, the solution at $t > t_0$ is:

$$\begin{aligned}
\Psi(x, t) &= \langle x | e^{-\frac{iH(t-t_0)}{\hbar}} | \Psi_0 \rangle \\
&= \int \langle x | e^{-\frac{iH(t-t_0)}{\hbar}} | y \rangle \langle y | \Psi_0 \rangle \, dy \\
&= \int K(x, t; y, t_0) \Psi_0(y) dy
\end{aligned} \tag{1.43}$$

- Having $K(x', t'; x, t)$, the solution to the Schrödinger equation is found by performing an integral.

- $K(x', t'; x, t)$ contains all the relevant information on the dynamics of the system.

1.2.2 The path integral computation for a free particle

Let us compute the propagator of a free particle, decribed by the lagrangian $\mathcal{L}(x, \dot{x}) = m\dot{x}^2/2$, using Feyman's time slicing procedure. Using the result of section 1.1.4 we can write

$$K(x_f, t_f; x_i, t_i) = \lim_{\epsilon \to 0} \frac{1}{A} \int \prod_{k=1}^{N-1} \frac{dx_k}{A} e^{\frac{iS}{\hbar}} \tag{1.44}$$

where:

$$\epsilon = \frac{t_f - t_i}{N}$$

$$S = \sum_{k=0}^{N-1} \frac{1}{2} m \frac{(x_{k+1} - x_k)^2}{\epsilon}$$

$$x_0 = x_i$$

$$x_N = x_f$$

Let us compute eq. (1.44) by integrating first over x_1. This coordinate only appears only in the first and the second time slice so we need just to concentrate on the integral

$$\begin{aligned}
&\int_{-\infty}^{\infty} dx_1 e^{i\frac{m}{2\epsilon\hbar}\left[(x_1 - x_0)^2 + (x_2 - x_1)^2\right]} \\
&= \int_{-\infty}^{\infty} dx_1 e^{i\frac{m}{2\epsilon\hbar}\left[2\left(x_1 - \frac{1}{2}(x_0 + x_2)\right)^2 + \frac{1}{2}(x_2 - x_0)^2\right]} \\
&= \underbrace{\sqrt{\frac{2\pi i\epsilon\hbar}{m}} \frac{1}{2}}_{A\sqrt{\frac{1}{2}}} e^{i\frac{m}{2\epsilon\hbar} \frac{1}{2}(x_2 - x_0)^2}
\end{aligned} \tag{1.45}$$

Notice that x_1 has disappeared: we "integrated it out" in the physics jargon. Putting this result back into eq. (1.44) we notice that we have an expression

similar to the original one but with $N - 1$ instead of N time slices. Moreover the first slice has now a width 2ϵ instead of ϵ: the factors of $1/2$ in both the exponent and prefactor of eq. (1.45) are checked to match this interpratation. It is now easy to go on. Let us do the integral on x_2 to gain more confidence. The relevant terms are

$$
\int_{-\infty}^{\infty} dx_2 e^{i\frac{m}{2\epsilon\hbar}\left[\frac{1}{2}(x_2-x_0)^2+(x_3-x_2)^2\right]}
$$

$$
= \int_{-\infty}^{\infty} dx_2 e^{i\frac{m}{2\epsilon\hbar}\left[\frac{3}{2}\left(x_2-\frac{1}{3}x_0-\frac{2}{3}x_3\right)^2+\frac{1}{3}(x_3-x_0)^2\right]}
$$

$$
= \underbrace{\sqrt{\frac{2\pi i\epsilon\hbar}{m}\frac{2}{3}}}_{A\sqrt{\frac{2}{3}}} e^{i\frac{m}{2\epsilon\hbar}\frac{1}{3}(x_3-x_0)^2} \tag{1.46}
$$

It is now clear how to proceed by induction. At the n-th step the integral over x_n will be:

$$
\int dx_n e^{i\frac{m}{2\epsilon\hbar}\left[\frac{1}{n}(x_n-x_0)^2+(x_{n+1}-x_n)^2\right]}
$$

$$
= \int dx_n e^{i\frac{m}{2\epsilon\hbar}\left[\frac{n+1}{n}\left(x_n-\left(\frac{1}{n+1}x_0+\frac{n}{n+1}x_{n+1}\right)\right)^2+\frac{1}{n+1}(x_{n+1}-x_0)^2\right]}
$$

$$
= \underbrace{\sqrt{\frac{2\pi i\epsilon\hbar}{m}\frac{n}{n+1}}}_{A\sqrt{\frac{n}{n+1}}} e^{i\frac{m}{2\epsilon\hbar}\frac{1}{n+1}(x_{n+1}-x_0)^2} \tag{1.47}
$$

Thus, putting all together, we find the expression of the propagator for a free particle:

$$
K(x_f,t_f;x_i,t_i) = \lim_{\epsilon\to 0}\frac{1}{A}\sqrt{\frac{1}{2}\frac{2}{3}\cdots\frac{N-1}{N}} e^{i\frac{m}{2\hbar N\epsilon}(x_f-x_i)^2} = \lim_{\epsilon\to 0}\frac{1}{A\sqrt{N}} e^{i\frac{m}{2\hbar N\epsilon}(x_f-x_i)^2}
$$

$$
= \sqrt{\frac{m}{2\pi i\hbar(t_f-t_i)}} e^{i\frac{m}{2\hbar}\frac{(x_f-x_i)^2}{t_f-t_i}} \tag{1.48}
$$

where we used the fact that $N\epsilon = t_f - t_i$.

We can check this result by computing directly the propagator of a one-dimensional free particle using the standard Hilbert space representation of the propagator:

$$
K(x_f,t;x_i,0) = \int \langle x_f|p\rangle \langle p| e^{-\frac{iHt}{\hbar}} |x_i\rangle \, dp
$$

$$
= \frac{1}{2\pi\hbar} \int e^{i\frac{p}{\hbar}(x_f-x_i)} e^{i\frac{p^2t}{2m\hbar}} \, dp
$$

$$
= \frac{1}{2\pi\hbar} \int e^{-\frac{it}{2m\hbar}\left(p-m\frac{x_f-x_i}{t}\right)^2+i\frac{m}{2\hbar}\frac{(x_f-x_i)^2}{t}} \, dp
$$

$$
= \sqrt{\frac{m}{2\pi i\hbar t}} e^{i\frac{m(x_f-x_i)^2}{2\hbar t}}
$$

$$
= F(t) e^{i\frac{S_{cl}(x_f,t;x_i,0)}{\hbar}} \tag{1.49}
$$

These results trivially generalize to the motion in higher dimensional spaces, as for the free particle the result factorizes.

- As we already saw, we can perform the same integral "à la Feynman" by dividing t into N infinitesimal steps.

- It is instructive interpret the result for the probability distribution:

$$\frac{dP}{dx} = |K|^2 = \frac{m}{2\pi\hbar t} \tag{1.50}$$

Let us interpret this result in terms of a flux of particles that started at $x_i = 0$ at $t = 0$ with a distribution of momenta

$$dn(p) = f(p)dp \tag{1.51}$$

and find what $f(p)$ is. A particle with momentum p at time t will have travelled to $x = (p/m)t$. Thus the particles in the interval dp will be at time t in the coordinate interval $dx = (t/m)dp$. Therefore we have $dn(x) = f(xm/t)(m/t)dx$. Comparing to (1.50), we find $f = 1/(2\pi\hbar) = const$. Thus, $dn(p) = (1/2\pi\hbar)dp \Rightarrow dn/dp \sim [\text{Length}]^{-1} \times [\text{Momentum}]^{-1}$. We recover the result that the wave function $\psi(x,t) = K(x,t;0,0)$ satisfies $\psi(x,0) = \delta(x)$ which corresponds in momentum space to an exactly flat distribution of momenta, with normalization $dn(p)/dp = (1/2\pi\hbar)$.

1.3 Path integrals as determinants

We will now introduce a systematic small $\hbar$ expansion for path integrals and show that the computation of the "leading" term in the expansion corresponds to the computation of the determinant of an operator. Before going to that, let us remind ourselves some basic results about "Gaussian" integrals in several variables.

1.3.1 Gaussian integrals

Let us give a look at gaussian integrals:

$$\int \prod_i dx_i e^{-\sum_{i,j} \lambda_{ij} x_i x_j} \tag{1.52}$$

- With one variable, and with λ real and positive we have:

$$\int dx e^{-\lambda x^2} = \sqrt{\frac{1}{\lambda}} \int dy e^{-y^2} = \sqrt{\frac{\pi}{\lambda}} \tag{1.53}$$

- Consider now a Gaussian integral with an arbitrary number of real variables

$$\int \prod_i dx_i e^{-\sum_{i,j} \lambda_{ij} x_i x_j} \tag{1.54}$$

where λ_{ij} is real.

We can rotate to the eigenbasis: $x_i = O_{ij}\tilde{x}_j$, with $O^T \lambda O = \text{diag}\,(\lambda_1, \ldots, \lambda_n)$, $O^T O = OO^T = 1$. Then, $\prod_i dx_i = |\det O| \prod_i d\tilde{x}_i = \prod_i d\tilde{x}_i$. Thus:

$$\int \prod_i dx_i e^{-\sum_{i,j} \lambda_{ij} x_i x_j} = \int \prod_i d\tilde{x}_i e^{-\sum_i \lambda_i \tilde{x}_i^2} =$$

$$\prod_i \sqrt{\frac{\pi}{\lambda_i}} = \sqrt{\frac{1}{\det(\frac{1}{\pi}\hat{\lambda})}} \quad (1.55)$$

where again the result makes sense only when all eigenvalues λ_n are positive.

- Along the same line we can consider integrals with imaginary exponents, which we indeed already encountered before

$$I = \int dx e^{i\lambda x^2} = e^{i\,\text{sgn}(\lambda)\frac{\pi}{4}} \sqrt{\frac{\pi}{|\lambda|}} \quad (1.56)$$

  This integral is performed by deforming the contour into the imaginary plane as discussed in homework 1. Depending on the sign of λ we must choose different contours to ensure convergence at infinity. Notice that the phase depends on the sign of λ.

- For the case of an integral with several variables

$$I = \int \prod_i dx_i e^{i \sum_{j,k} \lambda_{jk} x_j x_k} \quad (1.57)$$

  the result is generalized to

$$I = e^{i(n_+ - n_-)\frac{\pi}{4}} \sqrt{\frac{1}{|\det(\frac{1}{\pi}\hat{\lambda})|}} \quad (1.58)$$

  where n_+ and n_- are respectively the number of positive and negative eigenvalues of the matrix λ_{jk}.

1.3.2   Gaussian Path Integrals

Let us now make contact with the path integral:

$$K(x_f, t_f; x_i, t_i) = \int \mathscr{D}[x(t)] e^{i\frac{S[x(t)]}{\hbar}} \quad (1.59)$$

with

$$S[x(t)] = \int_{t_i}^{t_f} \mathcal{L}(x(t), \dot{x}(t)) dt \quad (1.60)$$

- To perform the integral, we can choose the integration variables that suit us best.

- The simplest change of variables is to shift $x(t)$ to "center" it around the classical solution $x_c(t)$:

$$x(t) = x_c(t) + y(t) \Rightarrow \mathscr{D}[x(t)] = \mathscr{D}[y(t)]$$

(the Jacobian for this change of variables is obviously trivial, as we indicated).

- We can Taylor expand $S[x_c(t) + y(t)]$ in $y(t)$ (note that $y(t_i) = y(t_f) = 0$, since the classical solution already satisfies the boundary conditions $x_c(t_i) = x_i$ and $x_c(t_f) = x_f$). By the usual definition of functional derivative, the Taylor expansion of a functional reads in general

$$
S[x_c(t) + y(t)] = S[x_c] + \int dt_1 \frac{\delta S}{\delta x(t_1)}\bigg|_{x=x_c} y(t_1) \tag{1.61}
$$
$$
+ \frac{1}{2} \int dt_1 dt_2 \frac{\delta^2 S}{\delta x(t_1)\delta x(t_2)}\bigg|_{x=x_c} y(t_1)y(t_2) + \mathcal{O}\left(y^3\right)
$$

with obvious generalization to all orders in y. In our case $S = \int dt \mathcal{L}(x, \dot{x})$ so that each term in the above general expansion can be written as a single dt integral

$$
\int dt_1 \frac{\delta S}{\delta x(t_1)}\bigg|_{x=x_c} y(t_1) \equiv \int dt \left\{ \frac{\partial \mathcal{L}}{\partial x}\bigg|_{x=x_c} y + \frac{\partial \mathcal{L}}{\partial \dot{x}}\bigg|_{x=x_c} \dot{y} \right\} \tag{1.62}
$$

$$
\frac{1}{2} \int dt_1 dt_2 \frac{\delta^2 S}{\delta x(t_1)\delta x(t_2)}\bigg|_{x=x_c} y(t_1)y(t_2) \equiv
$$
$$
\int dt \left\{ \frac{\partial^2 \mathcal{L}}{\partial x^2}\bigg|_{x=x_c} y^2 + 2\frac{\partial^2 \mathcal{L}}{\partial x \partial \dot{x}}\bigg|_{x=x_c} y\dot{y} + \frac{\partial^2 \mathcal{L}}{\partial \dot{x}^2}\bigg|_{x=x_c} \dot{y}^2 \right\} \tag{1.63}
$$

and so on.

The linear term in the expansion vanishes by the equations of motion:

$$
\int \frac{\delta S}{\delta x}\bigg|_{x=x_c} y(t)dt = \int \left(\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}} \right)\bigg|_{x=x_c} y(t)dt + \frac{\partial \mathcal{L}}{\partial \dot{x}}y(t)\bigg|_{t=t_i}^{t=t_f} = 0 \tag{1.64}
$$

Thus, we obtain the result:

$$
K(x_f, t_f; x_i, t_i) = \int \mathscr{D}[y(t)] e^{\frac{i}{\hbar}\left[S[x_c(t)] + \frac{1}{2}\frac{\delta^2 S}{\delta x^2}y^2 + \mathcal{O}(y^3) \right]} \tag{1.65}
$$

where $\delta^2 S/\delta x^2$ is just short hand for the second variation of S shown in eq. (1.63).
We can rewrite it rescaling our variables $y = \sqrt{\hbar}\,\tilde{y}$:

$$
K(x_f, t_f; x_i, t_i) = \mathcal{N} \cdot e^{\frac{i}{\hbar}S[x_c(t)]} \cdot \int \mathscr{D}[\tilde{y}(t)] e^{\frac{i}{2}\frac{\delta^2 S}{\delta x^2}\tilde{y}^2 + \mathcal{O}\left(\sqrt{\hbar}\,\tilde{y}^3\right)} \tag{1.66}
$$

where the overall constant $\mathcal{N}$ is just the Jacobian of the rescaling. [2] The interpretation of the above expression is that the quantum propagation of a particle can be decomposed into two pieces:

1. the <u>classical trajectory</u> $x_c(t)$, which gives rise to the exponent $e^{iS[x_c]/\hbar}$.

---

[2] Given that $\mathcal{N}$ is a constant its role is only to fix the right overall normalization of the propagator, and does not matter in assessing the relative importance of each trajectory. Therefore it does not play a crucial role in the following discussion.

2. the fluctuation $y(t)$ over which we must integrate; because of the quadratic term in the exponent, the path integral is dominated by $y \sim \mathcal{O}\left(\sqrt{\hbar}\right)$ (that is $\tilde{y} \sim \mathcal{O}(1)$) so that $y(t)$ represents the quantum fluctuation around the classical trajectory.

In those physical situations where $\hbar$ can be treated as a small quantity, one can treat $O(\hbar)$ in the exponent of the path integral as a perturbation

$$
\begin{aligned}
K(x_f, t_f; x_i, t_i) &= \mathcal{N} \cdot e^{\frac{i}{\hbar}S[x_c(t)]} \cdot \int \mathscr{D}[\tilde{y}(t)] e^{\frac{i}{2}\frac{\delta^2 S}{\delta x^2}\tilde{y}^2} \left[1 + \mathcal{O}(\hbar)\right] = (1.67)\\
&= F(x_f, t_f; x_i, t_i) e^{\frac{i}{\hbar}S[x_c(t)]} \left[1 + \mathcal{O}(\hbar)\right] \qquad (1.68)
\end{aligned}
$$

Where the prefactor F is just the gaussian integral around the classical trajectory. The semiclassical limit should thus correspond to the possibility to reduce the path integral to a gaussian integral. We will study this in more detail later on.

In the small $\hbar$ limit, the "classical" part of the propagator, $\exp(iS[x_c]/\hbar)$ oscillates rapidly when the classical action changes, while the prefactor (F and the terms in square brakets in eq. (1.68)) depend smoothly on $\hbar$ in this limit.

As an example, we can compute the value of S_{cl} for a simple macroscopic system: a ball weighing one gram moves freely along one meter in one second. We will use the following unity for energy: $[\text{erg}] = [\text{g}] \times ([\text{cm}]/[\text{s}])^2$.

$$
S_{cl} = \frac{1}{2}m\frac{(x_f - x_i)^2}{t_f - t_i} = \frac{1}{2}mv\Delta x = 5000 \text{ erg} \cdot \text{s}
$$

$$
\hbar = 1.0546 \cdot 10^{-27} \text{ erg} \cdot \text{s}
$$

$$
\Rightarrow S_{cl}/\hbar \sim 10^{30}
$$

1.3.3 $O(\hbar)$ corrections to Gaussian approximation

It is a good exercise to write the expression for the $O(\hbar)$ correction to the propagator K in eq. (1.68). In order to do so we must expand the action to order $\tilde{y}^4$ around the classical solution (using the same short hand notation as before for the higher order variation of S)

$$
\frac{S[x_c + \sqrt{\hbar}\tilde{y}]}{\hbar} = \frac{S[x_c]}{\hbar} + \frac{1}{2}\frac{\delta^2 S}{\delta x^2}\tilde{y}^2 + \frac{\sqrt{\hbar}}{3!}\frac{\delta^3 S}{\delta x^3}\tilde{y}^3 + \frac{\hbar}{4!}\frac{\delta^4 S}{\delta x^4}\tilde{y}^4 + O(\hbar^{3/2}) \quad (1.69)
$$

and then expand the exponent in the path integral to order $\hbar$. The leading $\hbar^{1/2}$ correction vanishes because the integrand is odd under $\tilde{y} \rightarrow -\tilde{y}$

$$
\int \mathscr{D}[\tilde{y}(t)] \frac{\sqrt{\hbar}}{3!}\frac{\delta^3 S}{\delta x^3}\tilde{y}^3 \, e^{\frac{i}{2}\frac{\delta^2 S}{\delta x^2}\tilde{y}^2} = 0 \qquad (1.70)
$$

and for the $O(\hbar)$ correction to K we find that two terms contribute

$$
\Delta K = i\hbar e^{\frac{i}{\hbar}S[x_c(t)]}\mathcal{N}\int \mathscr{D}[\tilde{y}(t)] \left\{\frac{1}{4!}\frac{\delta^4 S}{\delta x^4}\tilde{y}^4 + i\frac{1}{2}\left[\frac{1}{3!}\frac{\delta^3 S}{\delta x^3}\tilde{y}^3\right]^2\right\} e^{\frac{i}{2}\frac{\delta^2 S}{\delta x^2}\tilde{y}^2} \quad (1.71)
$$

1.3.4 Quadratic lagrangians and the harmonic oscillator

Consider now a special case: the quadratic lagrangians, defined by the property:

$$\frac{\delta^{(n)}S}{\delta x^n} = 0 \quad \text{for } n > 2 \tag{1.72}$$

For these lagrangians, the gaussian integral coresponds to the exact result:

$$K(x_f, t_f; x_i, t_i) = e^{i\frac{S[x_c]}{\hbar}} \int \mathscr{D}[y] e^{\frac{i}{\hbar}\frac{1}{2}\frac{\delta^2 S}{\delta x^2}y^2}$$

$$= const \cdot e^{i\frac{S[x_c]}{\hbar}} \left(\det \frac{\delta^2 S}{\delta x^2}\right)^{-\frac{1}{2}} \tag{1.73}$$

To make sense of the above we must define this strange "beast": the determinant of an operator. It is best illustrated with explicit examples, and usually computed indiretly using some "trick". This is a curious thing about path integrals: one never really ends up by computing them directly.

Let us compute the propagator for the harmonic oscillator using the determinant method. We have the lagrangian:

$$\mathcal{L}(x, \dot{x}) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 \tag{1.74}$$

It is left as an exercise to show that:

$$S_{cl} = \int_{t_i}^{t_f} \mathcal{L}(x_c, \dot{x}_c)dt = \frac{m\omega}{2}\left[\left(x_f{}^2 + x_i{}^2\right)\cot(\omega T) - \frac{2x_f x_i}{\sin(\omega T)}\right] \tag{1.75}$$

where $T = t_f - t_i$.

Then,

$$\int_{t_i}^{t_f} \mathcal{L}(x_c + y, \dot{x}_c + \dot{y})dt = \int_{t_i}^{t_f} \frac{1}{2}m\left(\dot{x}_c{}^2 - \omega^2 x_c{}^2\right)dt + \int_{t_i}^{t_f} \frac{1}{2}m\left(\dot{y}^2 - \omega^2 y^2\right)dt \tag{1.76}$$

And thus, the propagator is:

$$K(x_f, t_f; x_i, t_i) = e^{i\frac{S_{cl}}{\hbar}} \cdot \int \mathscr{D}[y] e^{\frac{i}{\hbar}\int_{t_i}^{t_f} \frac{m}{2}\left(\dot{y}^2 - \omega^2 y^2\right)dt}$$

$$= e^{i\frac{S_{cl}(x_f, x_i, t_f - t_i)}{\hbar}} \cdot J(t_f - t_i) \tag{1.77}$$

This is because $y(t)$ satisfies $y(t_i) = y(t_f) = 0$ and any reference to x_f and x_i has disappeared from the integral over y. Indeed J is just the propagator from $x_i = 0$ to $x_f = 0$:

$$K(x_f, t_f; x_i, t_i) = e^{i\frac{S_{cl}(x_f, x_i, t_f - t_i)}{\hbar}} \cdot \underbrace{K(0, t_f; 0, t_i)}_{J(t_f - t_i)} \tag{1.78}$$

We already have got a non trivial information by simple manipulations. The question now is how to compute $J(t_f - t_i)$.

1. Trick number 1: use the composition property of the transition amplitude:

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

Applying this to $J(t_f - t_i)$, we get:

$$J(t_f - t_i) = K(0, t_f; 0, t_i) =$$
$$J(t_f - t)J(t - t_i) \int e^{\frac{i}{\hbar}(S_{cl}(0,x,t_f-t)+S_{cl}(x,0,t-t_i))} dx \quad (1.79)$$

We can put the expression of the classical action in the integral, and we get ($T = t_f - t_i$, $T_1 = t_f - t$, $T_2 = t - t_i$):

$$\frac{J(T)}{J(T_1)J(T_2)} = \int dx e^{i\frac{m\omega}{2\hbar}\left[x^2(\cot(\omega T_1)+\cot(\omega T_2))\right]} =$$
$$\int dx e^{i\lambda x^2} = \sqrt{\frac{i\pi}{\lambda}} = \left[\frac{2i\pi\hbar}{m\omega}\frac{\sin(\omega T_1)\sin(\omega T_2)}{\sin(\omega T)}\right]^{\frac{1}{2}} \quad (1.80)$$

The general solution to the above equation is

$$J(T) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}} e^{aT} \quad (1.81)$$

with a an arbitrary constant. So this trick is not enough to fully fix the propagator, but it already tells us a good deal about it. We will now compute J directly and find $a = 0$. Notice that in the limit $\omega \to 0$, the result goes back to that for a free particle.

2. Now, let us compute the same quantity using the determinant method. What we want to compute is:

$$J(T) = \int \mathscr{D}[y] e^{\frac{i}{\hbar}\int_{t_i}^{t_f}\frac{m}{2}(\dot{y}^2-\omega^2 y^2)} \quad (1.82)$$

with the boundary conditions:

$$y(t_i) = y(t_f) = 0 \quad (1.83)$$

We can note the property:

$$i\int_{t_i}^{t_f}\frac{m}{2\hbar}(\dot{y}^2-\omega^2 y^2)\, dt = -i\int_{t_i}^{t_f}\frac{m}{2\hbar}y\left(\frac{d^2}{dt^2}+\omega^2\right)y\, dt = \frac{i}{2}\int_{t_i}^{t_f}y\hat{O}y\, dt \quad (1.84)$$

where $\hat{O} = -\frac{m}{\hbar}\left(\frac{d^2}{dt^2}+\omega^2\right)$.

Formally, we have to perform a gaussian integral, and thus the final result is proportional to $\left(\det\hat{O}\right)^{-1/2}$.

To make it more explicit, let us work in Fourier space for y:

$$y(t) = \sum_n a_n y_n(t) \quad (1.85)$$

where $y_n(t)$ are the othonormal eigenfunctions of $\hat{O}$:

$$y_n = \sqrt{\frac{2}{T}} \sin(\frac{n\pi}{T}t) \quad , n \in \mathbb{N}^* \tag{1.86}$$

$$\hat{O}y_n(t) = \lambda_n y_n(t) \tag{1.87}$$

$$\int y_n y_m dt = \delta_{nm} \tag{1.88}$$

The eigenvalues are

$$\lambda_n = \frac{m}{\hbar}\left[\left(\frac{n\pi}{T}\right)^2 - \omega^2\right] \tag{1.89}$$

Notice that the number of negative eigenvalues is finite and given by $n_- = \text{int}(\frac{T\omega}{\pi})$, that is the number of half periods of oscillation contained in T. The y_n form a complete basis of the Hilbert space $L_2([t_i, t_f]) \mod y(t_i) = y(t_f) = 0$. Thus, the a_n form a discrete set of integration variables, and we can write:

$$\mathscr{D}[y(t)] = \prod_n \frac{da_n}{\sqrt{2\pi i}} \cdot \underbrace{\tilde{N}}_{\text{``Jacobian''}} \tag{1.90}$$

where the $1/\sqrt{2\pi i}$ factors are singled out for later convenience (and also to mimick the $1/A$ factors in our definition of the measure in eq. (1.16)). We get:

$$\int y\hat{O}y\, dt = \sum_{m,n} \int a_m a_n y_m \hat{O}y_n dt = \sum_n \lambda_n a_n^2 \tag{1.91}$$

And thus,

$$
J(T) = \tilde{N} \int \prod_n \frac{da_n}{\sqrt{2\pi i}} e^{\frac{i}{2}\sum_n \lambda_n a_n^2} = \overbrace{\underbrace{\left(|\prod_n \lambda_n|\right)^{-\frac{1}{2}} \tilde{N}}_{\text{well defined}}}^{\text{ill defined}} \frac{e^{i(n_+ - n_-)\frac{\pi}{4}}}{e^{i(n_+ + n_-)\frac{\pi}{4}}}
$$

$$
= \left(|\prod_n \lambda_n|\right)^{-\frac{1}{2}} \tilde{N}\, e^{-in_-\frac{\pi}{2}} \tag{1.92}
$$

Notice that in the continuum limit $\epsilon \to 0$ in the definition of the measure eq. (1.16), we would have to consider all the Fourier modes with arbitrarily large n. In this limit both the product of eigenvalues and the Jacobian $\tilde{N}$ are ill defined. Their product however, the only physically relevant quantity, is well defined. We should not get into any trouble if we avoid computing these two quantities separately. The strategy is to work only with ratios that are well defined. That way we shall keep at large from mathematical difficulties (and confusion!), as we will now show.

Notice that $\hat{O}$ depends on ω, while $\tilde{N}$ obviously does not: the modes y_n do not depend on ω [3]. For $\omega = 0$, our computation must give the free

---

[3]Indeed a stronger result for the independence of the Jacobian on the quadratic action holds, as we shall discuss in section 3.1.

particle result, which we already know. So we have

$$J_\omega(T) = \tilde{N} \left(|\det \hat{O}_\omega| \right)^{-\frac{1}{2}} e^{-in-\frac{\pi}{2}} \tag{1.93}$$

$$J_0(T) = \tilde{N} \left(|\det \hat{O}_0| \right)^{-\frac{1}{2}} \tag{1.94}$$

We can thus consider

$$\frac{J_\omega(T)}{J_0(T)} e^{in-\frac{\pi}{2}} = \left(|\frac{\det \hat{O}_0}{\det \hat{O}_\omega}| \right)^{\frac{1}{2}} = \left(\frac{\prod_n |\lambda_n(\omega=0)|}{\prod_n |\lambda_n(\omega)|}| \right)^{\frac{1}{2}} = \left(|\prod_n \frac{\lambda_n(0)}{\lambda_n(\omega)}| \right)^{\frac{1}{2}} \tag{1.95}$$

The eigenvalues of the operator $\hat{O}_\omega = -\frac{m}{\hbar} \left(\frac{d^2}{dt^2} + \omega^2 \right)$ over the space of functions $y(t)$ have been given before:

$$\frac{\lambda_n(0)}{\lambda_n(\omega)} = \frac{\left(\frac{n\pi}{T} \right)^2}{\left(\frac{n\pi}{T} \right)^2 - \omega^2} = \frac{1}{1 - \left(\frac{\omega T}{n\pi} \right)^2} = \frac{1}{1 - \left(\frac{a}{n\pi} \right)^2} \tag{1.96}$$

$$\prod_{n=1}^\infty \frac{\lambda_n(0)}{\lambda_n(\omega)} = \prod_{n=1}^\infty \frac{1}{1 - \left(\frac{a}{n\pi} \right)^2} = \frac{a}{\sin a} \tag{1.97}$$

By eq. (1.95) we get our final result:

$$J_\omega(T) = J_0(T) \cdot \sqrt{\frac{\omega T}{|\sin(\omega T)|}} e^{-in-\frac{\pi}{2}} = \sqrt{\frac{m\omega}{2\pi i\hbar |\sin(\omega T)|}} e^{-in-\frac{\pi}{2}} \tag{1.98}$$

So that by using eq. (1.75) the propagator is (assume for simplicity $\omega T < \pi$)

$$K(x_f, T; x_i, 0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}} e^{i\frac{m\omega}{2\hbar} \left[\left(x_f{}^2 + x_i{}^2 \right) \cot(\omega T) - \frac{2x_f x_i}{\sin(\omega T)} \right]} \tag{1.99}$$

At this point, we can make contact with the solution of the eigenvalue problem and recover the well know result for the energy levels of the harmonic oscillator. Consider $\{\Psi_n\}$ a complete orthonormal basis of eigenvectors of the hamiltonian such that $H |\Psi_n\rangle = E_n |\Psi_n\rangle$. The propagator can be written as:

$$K(x_f, t_f; x_i, t_i) = \sum_{m,n} \langle x_f|\Psi_n\rangle \langle \Psi_n| e^{-\frac{iH(t_f - t_i)}{\hbar}} |\Psi_m\rangle \langle \Psi_m|x_i\rangle =$$

$$\sum_n \Psi_n^*(x_i)\Psi_n(x_f) e^{-\frac{iE_n(t_f - t_i)}{\hbar}} \tag{1.100}$$

Let us now define the partition function:

$$Z(t) = \int K(x, T; x, 0) dx = \sum_n \left(\int |\Psi_n(x)|^2 dx \right) e^{-\frac{iE_n T}{\hbar}} = \sum_n e^{-\frac{iE_n T}{\hbar}} \tag{1.101}$$

For the harmonic oscillator, using eq. (1.100) we find:

$$\int K(x, T; x, 0) dx = \frac{1}{2i\sin\left(\frac{\omega T}{2} \right)} = e^{-i\frac{\omega T}{2}} \frac{1}{1 - e^{-2i\frac{\omega T}{2}}} = \sum_{n=0}^\infty e^{-i(2n+1)\frac{\omega T}{2}} \tag{1.102}$$

$$\Rightarrow E_n = \hbar\omega \left(n + \frac{1}{2} \right) \tag{1.103}$$

1.4 Operator matrix elements

We will here derive the matrix elements of operators in the path integral formalism.

1.4.1 The time-ordered product of operators

Let us first recall the basic definition of quantities in the Heisenberg picture. Given an operator $\hat{O}$ in the Schroedinger picture, the time evolved Heisenberg picture operator is

$$\hat{O}(t) \equiv e^{iHt} \hat{O} e^{-iHt} . \tag{1.104}$$

In particular for the position operator we have

$$\hat{x}(t) \equiv e^{iHt} \hat{x} e^{-iHt} . \tag{1.105}$$

Given a time the independent position eigenstates $|x\rangle$, the vectors

$$|x, t\rangle \equiv e^{iHt} |x\rangle \tag{1.106}$$

represent the basis vectors in the Heisenberg picture (notice the "+" in the exponent as opposed to the "−" in the evolution of the state vector in the Schroedinger picture!), being eigenstates of $\hat{x}(t)$

$$\hat{x}(t) |x, t\rangle = x |x, t\rangle . \tag{1.107}$$

We have the relation:

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathscr{D}[x(t)] e^{i \frac{S[x(t)]}{\hbar}} . \tag{1.108}$$

By working out precisely the same algebra which we used in section
 Consider now a function $A(x)$. It defines an operator on the Hilbert space:

$$\hat{A}(\hat{x}) \equiv \int |x\rangle \langle x| A(x) dx \tag{1.109}$$

Using the factorization property of the path integral we can derive the following identity:

$$\int \mathscr{D}[x] A(x(t_1)) e^{i \frac{S[x]}{\hbar}} =$$
$$\int \mathscr{D}[x_a] \mathscr{D}[x_b] dx_1 A(x_1) e^{i \frac{S[x_a] + S[x_b]}{\hbar}} =$$
$$\int dx_1 \langle x_f | e^{-\frac{iH(t_f - t_1)}{\hbar}} |x_1\rangle \langle x_1 | e^{-\frac{iH(t_1 - t_i)}{\hbar}} |x_i\rangle A(x_1) =$$
$$\langle x_f | e^{-\frac{iH(t_f - t_1)}{\hbar}} \hat{A}(\hat{x}) e^{-\frac{iH(t_1 - t_i)}{\hbar}} |x_i\rangle =$$
$$\langle x_f | e^{-\frac{iHt_f}{\hbar}} \hat{A}(\hat{x}(t_1)) e^{\frac{iHt_i}{\hbar}} |x_i\rangle =$$
$$\langle x_f, t_f | \hat{A}(\hat{x}(t_1)) |x_i, t_i\rangle \tag{1.110}$$

Let us now consider two functions $O_1(x(t))$ and $O_2(x(t))$ of $x(t)$ and let us study the meaning of:

$$\int \mathscr{D}[x] O_1(x(t_1)) O_2(x(t_2)) e^{i\frac{S[x]}{\hbar}} \tag{1.111}$$

By the composition property, assuming that $t_1 < t_2$, we can equal it to (see figure 1.8):

$$\int \mathscr{D}[x_a] \mathscr{D}[x_b] \mathscr{D}[x_c] dx_1 dx_2 e^{i\frac{S[x_a]+S[x_b]+S[x_c]}{\hbar}} O_2(x_2) O_1(x_1) \tag{1.112}$$
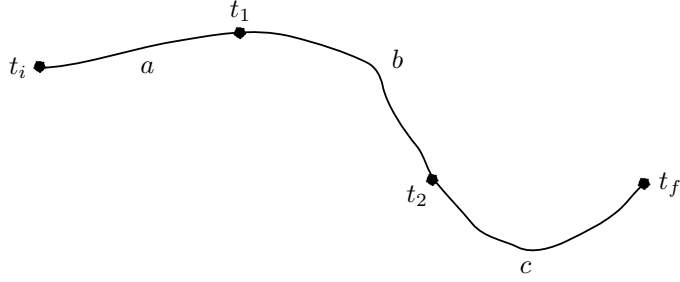

Figure 1.8: The path from (x_i, t_i) to (x_f, t_f) is separated into three paths a, b and c. We have to distinguish $t_1 < t_2$ from $t_2 < t_1$.

This can be rewritten:

$$\int \langle x_f, t_f | x_2, t_2 \rangle O_2(x_2) \langle x_2, t_2 | x_1, t_1 \rangle O_1(x_1) \langle x_1, t_1 | x_i, t_i \rangle dx_2 dx_1 \tag{1.113}$$

Using the equation (1.109), it can be rewritten:

$$\langle x_f | e^{-\frac{iH(t_f-t_2)}{\hbar}} \hat{O}_2(\hat{x}) e^{-\frac{iH(t_2-t_1)}{\hbar}} \hat{O}_1(\hat{x}) e^{-\frac{iH(t_1-t_i)}{\hbar}} | x_i \rangle =$$
$$\langle x_f, t_f | \hat{O}_2(t_2) \hat{O}_1(t_1) | x_i, t_i \rangle \tag{1.114}$$

Recall that this result is only valid for $t_2 > t_1$.

Exercise: Check that for $t_1 > t_2$, one gets instead:

$$\langle x_f, t_f | \hat{O}_1(t_1) \hat{O}_2(t_2) | x_i, t_i \rangle \tag{1.115}$$

Thus, the final result is:

$$\int \mathscr{D}[x] O_1(x(t_1)) O_2(x(t_2)) e^{i\frac{S[x]}{\hbar}} = \langle x_f, t_f | T[\hat{O}_1(t_1) \hat{O}_2(t_2)] | x_i, t_i \rangle \tag{1.116}$$

where the time-ordered product $T[\hat{O}_1(t_1) \hat{O}_2(t_2)]$ is defined as:

$$T[\hat{O}_1(t_1) \hat{O}_2(t_2)] = \theta(t_2 - t_1) \hat{O}_2(t_2) \hat{O}_1(t_1) + \theta(t_1 - t_2) \hat{O}_1(t_1) \hat{O}_2(t_2) \tag{1.117}$$

where $\theta(t)$ is the Heaviside step function.

Exercise: Consider a system with classical Lagrangian $\mathcal{L} = m\frac{\dot{x}^2}{2} - V(x)$. Treating V as a perturbation and using the path integral, derive the well-known formula for the time evolution operator in the interaction picture

$$U(t) = e^{-iH_0 t/\hbar} \, \hat{T}[e^{-\frac{i}{\hbar}\int_0^t \hat{V}(t',\hat{x})dt'}] \tag{1.118}$$

where $H_0 = \frac{\hat{p}^2}{2m}$ and $\hat{V}(t,\hat{x}) = e^{iH_0 t/\hbar} V(\hat{x}) e^{-iH_0 t/\hbar}$.

Chapter 2

Functional and Euclidean methods

In this chapter, we will introduce two methods:

- The functional method, which allows a representations of perturbation theory in terms of Feynman diagrams.

- The Euclidean path integral, which is useful for, e.g., statistical mechanics and semiclassical tunneling.

We will show a common application of both methods by finding the perturbative expansion of the free energy of the anharmonic oscillator.

2.1 Functional method

Experimentally, to find out the properties of a physical system (for example an atom), we let it interact with an external perturbation (a source, e.g. an electromagnetic wave), and study its response.

This basic empirical fact has its formal counterpart in the theoretical study of (classical and) quantum systems.

To give an illustration, let us consider a system with Lagrangian $\mathcal{L}(x, \dot{x})$ and let us make it interact with an arbitrary external forcing source:

$$\mathcal{L}(x, \dot{x}) \to \mathcal{L}(x, \dot{x}) + J(t)x(t)$$

$$K(x_f, t_f; x_i, t_i | J) = \int \mathscr{D}[x] e^{\frac{i}{\hbar} \int (\mathcal{L}(x, \dot{x}) + J(t)x(t))dt} \tag{2.1}$$

K has now become a functional of $J(t)$. This functional contains important physical information about the system (all information indeed) as exemplified by the fact that the functional derivatives of K give the expectation values of $\hat{x}$ (and thus of all operators that are a function of x):

$$\frac{\hbar\delta}{i\delta J(t_1)} \cdots \frac{\hbar\delta}{i\delta J(t_n)} K(x_f, t_f; x_i, t_i | J)\Big|_{J=0} = \langle x_f, t_f | T[\hat{x}(t_1), \ldots, \hat{x}(t_n)] | x_i, t_i \rangle \tag{2.2}$$

As an example, let us see how the effects of a perturbation can be treated with functional methods.

Let us look at the harmonic oscillator, with an anharmonic self-interaction which is assumed to be small enough to be treated as a perturbation:

$$\mathcal{L}_0(x, \dot{x}) = \frac{m}{2}\dot{x}^2 - \frac{m\omega^2}{2}x^2, \quad \mathcal{L}_{pert}(x, \dot{x}) = -\frac{\lambda}{4!}x^4 \tag{2.3}$$

The propagator $K_0[J]$ for the harmonic oscillator with a source $J(t)$ is:

$$K_0[J] = \int \mathscr{D}[x] e^{\frac{i}{\hbar}\int(\mathcal{L}_0 + J(t)x(t))dt} \tag{2.4}$$

Consider now the addition of the perturbation. By repeated use of the functional derivatives with respect to J (see eq. (2.2)) the propagator can be written as:

$$
\begin{aligned}
K[J] &= \int \mathscr{D}[x] e^{\frac{i}{\hbar}\int\left(\mathcal{L}_0 - \frac{\lambda}{4!}x^4 + J(t)x(t)\right)dt} \\
&= \int \mathscr{D}[x] \sum_n \frac{1}{n!} \int \left(\frac{-i\lambda}{\hbar 4!}\right)^n x^4(t_1) \cdots x^4(t_n) e^{\frac{i}{\hbar}\int(\mathcal{L}_0 + J(t)x(t))dt} dt_1 \cdots dt_n \\
&= \sum_n \frac{1}{n!} \int \left(\frac{-i\lambda}{\hbar 4!}\right)^n \frac{\hbar^4 \delta^4}{\delta J^4(t_1)} \cdots \frac{\hbar^4 \delta^4}{\delta J^4(t_n)} K_0[J] dt_1 \cdots dt_n \\
&\equiv \exp\left(-\int dt \frac{i\lambda\hbar^3}{4!}\frac{\delta^4}{\delta J^4(t)}\right) K_0[J]
\end{aligned}
\tag{2.5}
$$

Thus, when we take the $J \to 0$ limit, we get the propagator of the anharmonic hamiltonian in terms of functional derivatives of the harmonic propagator in presence of an arbitrary source J.

2.2   Euclidean Path Integral

Instead of computing the transition amplitude $\langle x_f | e^{-\frac{iHt}{\hbar}} | x_i \rangle$, we could have computed the imaginary time evolution:

$$K_E \equiv \langle x_f | e^{-\frac{\beta H}{\hbar}} | x_i \rangle, \quad \beta \in \mathbb{R}_+ \tag{2.6}$$

which corresponds to an imaginary time interval $t = -i\beta$.
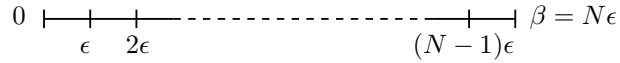

Figure 2.1: The interval between 0 and β is divided into N steps.

It is straightforward to repeat the same time slicing procedure we employed in section 1.1.4 (see figure 2.1) and write the imaginary time amplitude as a path integral. The result is:

$$K_E(x_f, x_i; \beta) = \int \mathscr{D}[x]_E e^{-\frac{1}{\hbar}S_E[x]} \tag{2.7}$$

where $D[x]_E$ is a path integration measure we shall derive below and where

$$S_E[x] = \int_0^\beta \left(\frac{m}{2} \left(\frac{dx}{d\tau} \right)^2 + V(x) \right) d\tau \sim \beta E \qquad (2.8)$$

Notice that S_E is normally minimized on stationary points.

From a functional viewpoint K_E is the continuation of K to the imaginary time axis

$$K_E(x_f, x_i; \beta) = K(x_f, x_i; -i\beta). \qquad (2.9)$$

Notice that more sloppily we could have also gotten K_E by "analytic continuation" to imaginary time directly in the path integral:

$$K(t) = \int \mathscr{D}[x] e^{\frac{i}{\hbar} \int_0^t \mathcal{L}(x, \dot{x}) dt'} \qquad (2.10)$$

Then, with the following replacements

$$t' = -i\tau$$
$$dt' = -id\tau$$
$$\dot{x} = i\frac{dx}{d\tau}$$
$$t = -i\beta$$

we obviously get the same result. Notice that the proper time interval in the relativistic description $ds^2 = -dt^2 + dx_i^2$, corresponding to a Minkovsky metric with signature $-, +, +, +$, gets mapped by going to imaginary time into a metric with Euclidean signature $ds_E^2 = d\tau^2 + dx_i^2$. Hence the 'Euclidean' suffix.

Let us now compute explicitly by decomposing the imaginary time interval $[0, \beta]$ into N steps of equal length ϵ (see figure 2.1). As in section 1.1.4 we can write:

$$K_E(x_f, x_i; \beta) = \int \langle x_N | e^{-\frac{H\epsilon}{\hbar}} | x_{N-1} \rangle \cdots \langle x_1 | e^{-\frac{H\epsilon}{\hbar}} | x_0 \rangle dx_1 \cdots dx_{N-1} \qquad (2.11)$$

where $x_f = x_N$ and $x_i = x_0$.

We can compute, just as before:

$$\langle x' | e^{-\frac{H\epsilon}{\hbar}} | x \rangle = \int \langle x' | p \rangle \langle p | e^{-\frac{H\epsilon}{\hbar}} | x \rangle dp$$

$$\approx \frac{1}{2\pi\hbar} \int e^{\frac{ip}{\hbar}(x'-x) - \frac{\epsilon}{\hbar}\left(\frac{p^2}{2m} + V(x) \right)} dp$$

$$= \frac{1}{2\pi\hbar} \int e^{-\frac{\epsilon}{2m\hbar}\left(p - i\frac{m}{\epsilon}(x'-x) \right)^2 - \frac{m}{2\epsilon\hbar}(x'-x)^2 - \frac{\epsilon}{\hbar}V(x)} dp$$

$$= \sqrt{\frac{m}{2\pi\epsilon\hbar}} e^{-\frac{1}{\hbar}\left[\frac{m}{2}\left(\frac{x'-x}{\epsilon} \right)^2 + V(x) \right]\epsilon}$$

$$= \sqrt{\frac{m}{2\pi\epsilon\hbar}} e^{-\frac{1}{\hbar}\mathcal{L}_E(x,x')\epsilon} \equiv \frac{1}{A_E} e^{-\frac{S_E(x',x)}{\hbar}} \qquad (2.12)$$

and then proceed to obtain the Euclidean analogue of eq. (1.16)

$$K_E(x_f, x_i; \beta) = \lim_{\epsilon \to 0} \int \prod_{k=1}^{N-1} dx_k \frac{1}{A_E^N} e^{\frac{1}{\hbar} \sum_{l=0}^{N-1} S_E(x_{l+1}, x_l)}$$

$$= \lim_{\epsilon \to 0} \frac{1}{A_E} \int \underbrace{\prod_{k=1}^{N-1} \frac{dx_k}{A_E}}_{\int D[x]_E} e^{-\frac{S_E(x_f, x_i)}{\hbar}} \tag{2.13}$$

Synthetizing: to pass from the real time path integral formulation to the Euclidean time formulation, one simply makes the change $i\epsilon \to \epsilon$ in the factor A defining the measure of integration, and modifies the integrand according to

$$iS = i \int_0^t \left(\frac{1}{2} m \dot{x}^2 - V(x) \right) dt \longrightarrow -S_E = - \int_0^\beta \left(\frac{1}{2} m \dot{x}^2 + V(x) \right) d\tau$$

$$e^{iS/\hbar} \longrightarrow e^{-S_E/\hbar} \tag{2.14}$$

2.2.1   Statistical mechanics

Recalling the result of the previous section we have

$$K_E(x_f, x_i; \beta) = \sum_n \Psi_n^*(x_f) \Psi_n(x_i) e^{-\beta E_n / \hbar} \tag{2.15}$$

where $\{\Psi_n\}$ is an othonormal basis of eigenvectors of the Hamiltonian. We can then define the partition function:

$$Z[\beta] = \int dx K_E(x, x; \beta) = \sum_n e^{-\beta E_n / \hbar} \tag{2.16}$$

We recognize here the statistical mechanical definition of the thermal partition function for a system at temperature $k_B T = \hbar / \beta$, where k_B is the Boltzmann constant.

We can observe the equivalence:

$$Z[\beta] = \int dx K_E(x, x; \beta) = \int_{\{x(0) = x(\beta)\}} \mathscr{D}[x] e^{-S_E} \tag{2.17}$$

Thus, the thermal partition function is equivalent to a functional integral over a compact Euclidean time: $\tau \in [0, \beta]$ with boundaries identified. The integration variables $x(\tau)$ are therefore periodic in τ with period β.

Let us now check that $K(-i\beta)$ leads to the right partition function for the harmonic oscillator. Using equation (1.102), we get:

$$Z[\beta] = \int K(x, x; -i\beta) dx = \sum_n e^{-\beta \omega \left(n + \frac{1}{2} \right)} \tag{2.18}$$

which is indeed the expected result.

2.3 Perturbation theory

The purpose of this section is to illustrate the use of functional methods in the euclidean path integral. We shall do so by focussing on the anharmonic oscillator and by computing in perturbation theory the following physically relevant quantities

- the time ordered correlators on the ground state: $\langle 0|T[\hat{x}(\tau_1)\ldots\hat{x}(\tau_n)]|0\rangle$

- the free energy and the ground state energy.

2.3.1 Euclidean n-point correlators

Consider the euclidean path integral defined between initial time $\tau_i = -\frac{\beta}{2}$ and final time $\tau_f = +\frac{\beta}{2}$. As we did for the real time path integral, we can consider the euclidean n-point correlator

$$\int_{x(-\frac{\beta}{2})=x_i}^{x(\frac{\beta}{2})=x_f} \mathscr{D}[x(\tau)]_E \, x(\tau_1)\ldots x(\tau_n) e^{-\frac{S_E[x(\tau)]}{\hbar}} \tag{2.19}$$

By working out precisely the same algebra of section 1.4, the euclidean correlator is also shown to be equal to the operatorial expression

$$\langle x_f|e^{-\beta H/2\hbar}T[\hat{x}_E(\tau_1)\ldots\hat{x}_E(\tau_n)]e^{-\beta H/2\hbar}|x_i\rangle \tag{2.20}$$

where

$$\hat{x}_E(\tau) = e^{H\tau/\hbar}\hat{x}e^{-H\tau/\hbar} \tag{2.21}$$

represents the continuation to imaginary time of the Heisenberg picture position operator. Indeed, comparing to eq. (1.105) we have, $\hat{x}_E(\tau) = \hat{x}(-i\tau)$.

It is interesting to consider the limit of the euclidean path integral and correlators when $\beta \to \infty$. This is most directly done by working in the operator formulation. By using the complete set of energy eigenstatets the euclidean amplitude can be written as

$$
\begin{aligned}
K_E(x_f, \frac{\beta}{2}; x_i, -\frac{\beta}{2}) &= \langle x_f|e^{-\frac{\beta H}{\hbar}}|x_i\rangle = \\
&= \sum_n \psi_n(x_f)\psi_n(x_i)^* e^{-\beta E_n/\hbar} \\
&\overset{\beta\to\infty}{=} \psi_0(x_f)\psi_0(x_i)^* e^{-\beta E_0/\hbar}\left[1 + O(e^{-\beta(E_1-E_0)\hbar})\right]
\end{aligned}
\tag{2.22}
$$

where E_0 and E_1 are the energies of respectively the ground state and the first excited state. From the above we conclude that for $\beta \gg \hbar/(E_1 - E_0)$ the operator $e^{-\beta H/\hbar}$ acts like a projector on the ground state. We arrive at the same conclusion also for the correlators

$$\lim_{\beta\to\infty}\langle x_f|e^{-\frac{\beta H}{2\hbar}}T[\hat{x}_E(\tau_1)\ldots\hat{x}_E(\tau_n)]e^{-\frac{\beta H}{2\hbar}}|x_i\rangle \tag{2.23}$$

$$=\langle 0|T[\hat{x}_E(\tau_1)\ldots\hat{x}_E(\tau_n)]|0\rangle \, \psi_0(x_f)\psi_0(x_i)^* e^{-\frac{\beta E_0}{\hbar}}\left[1 + O(e^{-\beta(E_1-E_0)/\hbar})\right]$$

where by $|0\rangle$ we indicate the energy ground state (not the $x = 0$ position eigenstate!). By taking the ratio of eq. (2.23) and eq. (2.22) we thus find

$$\lim_{\beta \to \infty} \frac{\langle x_f | e^{-\frac{\beta H}{2\hbar}} T[\hat{x}_E(\tau_1) \dots \hat{x}_E(\tau_n)] e^{-\frac{\beta H}{2\hbar}} | x_i \rangle}{\langle x_f | e^{-\frac{\beta H}{\hbar}} | x_i \rangle} = \langle 0 | T[\hat{x}_E(\tau_1) \dots \hat{x}_E(\tau_n)] | 0 \rangle$$

(2.24)

where the dependence on x_i and x_f has cancelled out. The time ordered correlators on the ground state are also known as Feynman correlators. Using the path integral fomulation we can suggestively write

$$\langle 0 | T[\hat{x}_E(\tau_1) \dots \hat{x}_E(\tau_n)] | 0 \rangle = \lim_{\beta \to \infty} \frac{\int \mathscr{D}[x(\tau)]_E \, x(\tau_1) \dots x(\tau_n) e^{-\frac{S_E}{\hbar}}}{\int \mathscr{D}[x(\tau)]_E e^{-\frac{S_E}{\hbar}}}$$

(2.25)

Notice that the structure of above equation is reminiscent of thermal averages in classical statistical mechanics, with the denominator playing the role of a partition function. As we already said, in the $\beta \to \infty$ limit the above equation is independent of x_i, x_f. For the sake simplicity we shall then focus on the case $x_i = x_f = 0$ and define, at finite β, the normalized n-point correlator as

$$\hbar^{\frac{n}{2}} G_D(\tau_1, \dots, \tau_n) = \frac{\int_{x_i = x_f = 0} \mathscr{D}[x(\tau)]_E \, x(\tau_1) \dots x(\tau_n) e^{-\frac{S_E}{\hbar}}}{\int_{x_i = x_f = 0} \mathscr{D}[x(\tau)]_E e^{-\frac{S_E}{\hbar}}}$$

(2.26)

where the suffix D indicates that this normalized n-point correlator was computed by imposing Dirichlet boundary conditions $x_i = x_f = 0$ in the path integral. In the definition of G_D, $\hbar^{n/2}$ is factored out for later convenience.

The euclidan Feynman correlators are related to the Feynman correlators in real time

$$\langle 0 | T[\hat{x}(t_1) \dots \hat{x}(t_n)] | 0 \rangle$$

(2.27)

by performing an analytic continuation $\tau_i \to it_i$ in such a way as to preserve the time ordering. This is most simply done via a counter-clockwise rotation, the Wick rotation, in the complex time plane as shown in fig. 2.2. Indeed the time ordered correlators, both for real and imaginary time, are by construction analytic functions of the time coordinates over the connected domains where none of the time coordinates (ex. τ_1, τ_2, $\dots$, τ_n) coincide. Each such domain corresponds to a give ordering of the n time coordinates. The non-analiticity is purely due to the step functions that enforce time ordering and is localized at the points where at least two coordinates coincide. Then by continuing the time coodinates on trajectories that do not cross (like in the Wick rotation) one remains within the domain of analyticity.

The real time Feynman correlators play an important role in relativistic quantum field theory. The n-point correlators are associated to the amplitudes describing the scattering of n_I initial particles into n_F final particles with $n = n_I + n_F$.

2.3.2   Thermal n-point correlators

One can also define the correlators using the path integral with periodic boundary conditions

$$\int_{x(-\frac{\beta}{2}) = x(\frac{\beta}{2})} \mathscr{D}[x(\tau)]_E \, x(\tau_1) \dots x(\tau_n) e^{-\frac{S_E[x(\tau)]}{\hbar}} \, .$$
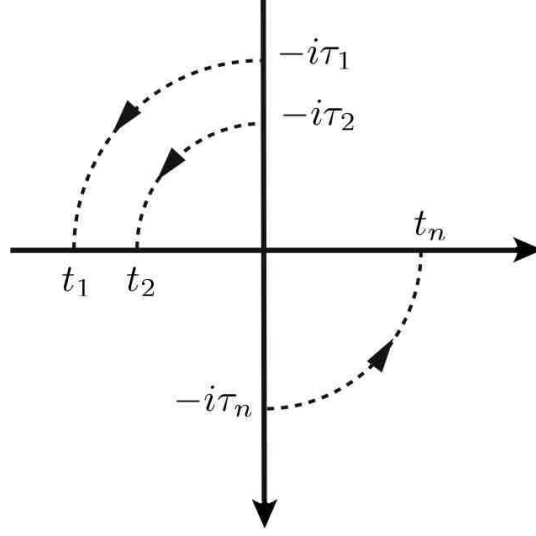
(2.28)

Figure 2.2: Wick rotation from imaginary to real time. The arrows on the coordinate axes indicate the future direction, both for real and imaginary time

This object should expectedly be related to statistical mechanics. Indeed, in the operator formulation, eq. (2.28) can be written as

$$\int \langle x|e^{-\frac{\beta H}{2\hbar}} T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]e^{-\frac{\beta H}{2\hbar}}|x\rangle dx = \mathrm{Tr}\left\{ e^{-\frac{\beta H}{\hbar}}[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\right\}$$
(2.29)

Normalizing by the partition function $Z = \mathrm{Tr}[e^{-\beta H/\hbar}]$ we obtain he thermal average of the time ordered operator product $T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]$

$$\langle T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\rangle_\beta = \frac{1}{Z(\beta)}\mathrm{Tr}\left\{ e^{-\frac{\beta H}{\hbar}} T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\right\} \qquad (2.30)$$

which in the path integral language corresponds to the normalized n-point thermal correlator

$$(2.30) = \frac{\int_{x(-\frac{\beta}{2})=x(\frac{\beta}{2})} \mathscr{D}[x(\tau)]_E\, x(\tau_1)\dots x(\tau_n)e^{-\frac{S_E}{\hbar}}}{\int_{x(-\frac{\beta}{2})=x(\frac{\beta}{2})} \mathscr{D}[x(\tau)]_E\, e^{-\frac{S_E}{\hbar}}} \equiv \hbar^{\frac{n}{2}} G_P(\tau_1,\dots,\tau_n)$$
(2.31)

where the have defined G_P in analogy with the Dirichlet n-point correlator of the previous section. G_D and G_P only differ by the choice of boundary conditions, respectively Dirichlet for G_D and periodic for G_P, applied to the corresponding path integrals.

Like with G_D, by performing the Wick rotation $\tau_k \to it_k$ we obtain

$$\hbar^{\frac{n}{2}} G_P(it_1,\dots,it_n) = \frac{1}{Z(\beta)}\mathrm{Tr}\left\{ e^{-\frac{\beta H}{\hbar}} T[\hat{x}(t_1)\dots\hat{x}(t_n)]\right\}, \qquad (2.32)$$

that is the thermal average of the time ordered product in real time.

Finally, notice that for $\beta \to \infty$ we have

$$\lim_{\beta \to \infty} \frac{e^{-\frac{\beta H}{\hbar}}}{Z(\beta)} = |0\rangle\langle 0| \tag{2.33}$$

This is expected, as $\beta \to \infty$ corresponds to a statistical ensemble at zero temperature. Then at $\beta \to \infty$ both Dirichlet and periodic correlators coincide with the Feynman correlator

$$\lim_{\beta \to \infty} \hbar^{\frac{n}{2}} G_P(\tau_1, \dots \tau_n) = \lim_{\beta \to \infty} \hbar^{\frac{n}{2}} G_D(\tau_1, \dots \tau_n) = \langle 0|T[\hat{x}_E(\tau_1) \dots \hat{x}_E(\tau_n)]|0\rangle . \tag{2.34}$$

From the path integral viewpoint, the coincidence of G_D and G_P in the above equation represents the expected fact that for finite $\tau_1, \dots, \tau_n$ the boundary conditions in eqs. (2.26,2.31) become irrelevant for $\beta \to \infty$

2.3.3   Euclidean correlators by functional derivatives

Consider the euclidean path integral for our system coupled to an external source $J(\tau)$. For the case of Dirichlet boundary conditions $x_i = x_f = 0$ we define

$$K_E[\beta, J] \equiv K_E(0, \frac{\beta}{2}; 0, -\frac{\beta}{2}|J) =$$
$$\int_{x_i=x_f=0} \mathscr{D}[x]_E \exp\left[-\frac{1}{\hbar} \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau \left(\mathcal{L}_E(x, \dot{x}) - J(\tau)x(\tau)\right)\right] \tag{2.35}$$

and similarly for periodic boundary conditions

$$Z[\beta, J] \equiv K_E(0, \frac{\beta}{2}; 0, -\frac{\beta}{2}|J) =$$
$$\int_{x_i=x_f} \mathscr{D}[x]_E \exp\left[-\frac{1}{\hbar} \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau \left(\mathcal{L}_E(x, \dot{x}) - J(\tau)x(\tau)\right)\right] . \tag{2.36}$$

The correlators can then be expressed in terms of functional derivatives. Using the definitions in eqs. (2.26,2.31) we have

$$\hbar^{\frac{n}{2}} G_D(\tau_1, \dots, \tau_n) = \frac{1}{K_E[\beta, 0]} \frac{\hbar\delta}{\delta J(\tau_1)} \dots \frac{\hbar\delta}{\delta J(\tau_n)} K_E[\beta, J]\Big|_{J=0} \tag{2.37}$$

$$\hbar^{\frac{n}{2}} G_P(\tau_1, \dots, \tau_n) = \frac{1}{Z[\beta, 0]} \frac{\hbar\delta}{\delta J(\tau_1)} \dots \frac{\hbar\delta}{\delta J(\tau_n)} Z[\beta, J]\Big|_{J=0} \tag{2.38}$$

Like in section 2.1 we define $K_E^0[\beta, J]$ and $Z^0[\beta, J]$ to be the path integrals associated to the simple harmonic oscillator with euclidean lagrangian $\mathcal{L}_E^0 = \frac{m\dot{x}^2}{2} + \frac{m\omega^2 x^2}{2}$. We want to consider the general anharmonic oscillator with lagrangian

$$\mathcal{L}_E = \frac{m\dot{x}^2}{2} + \frac{m\omega^2 x^2}{2} + \Delta V(x) = \mathcal{L}_E^0 + \Delta V(x) \tag{2.39}$$

where ΔV can be treated as a small perturbation of the dynamics of $\mathcal{L}_E^0$. Again just following the procedure shown in section 2.1, the path integrals for the

anharmonic oscillator can be written as

$$K_E[\beta, J] \;=\; \exp\left[-\frac{1}{\hbar}\int d\tau\, \Delta V\Big(\frac{\hbar\delta}{\delta J(\tau)}\Big)\right] K_E^0[\beta, J] \tag{2.40}$$

$$Z[\beta, J] \;=\; \exp\left[-\frac{1}{\hbar}\int d\tau\, \Delta V\Big(\frac{\hbar\delta}{\delta J(\tau)}\Big)\right] Z^0[\beta, J] \tag{2.41}$$

Summarizing: to compute any interesting quantity (correlator or partition function) we must

1. compute the unperturbed K_E^0 and Z^0,

2. learn to take their derivatives with respect to $J(\tau)$ in an efficient way.

The first step amounts to a Gaussian integral. The second is basically a problem in combinatorics, whose solution has a convenient diagrammatic representation: the Feynman diagrams.

2.3.4 Computing $K_E^0[J]$ and $Z^0[J]$

$K_E^0[\beta, J]$ and $Z^0[\beta, J]$ are just gaussian integrals with an external source (euclidean forced harmonic oscillator). To compute them we can use the method of Green's functions.

First, let us recall the result for a gaussian integral with a linear source (in the discrete finite case). We want to compute the integral:

$$I[J] = \int \prod_k^n dx_k\, e^{-\frac{1}{2}x^i O_{ij} x^j + J_k x^k} \tag{2.42}$$

where O_{ij} is a positive definite $n \times n$ matrix and we sum over repeated indices.

The inverse G of the matrix O is defined by:

$$G^{ij} O_{jk} = O_{kj} G^{ji} = \delta^i{}_k \tag{2.43}$$

Such an inverse matrix exists, since O_{ij} is assumed positive definite. We then perform the change of variables $\bar{x}^i = x^i - G^{ij} J_j$ which obviously has trivial Jacobian

$$\prod_k dx_k = \prod_k d\bar{x}_k \tag{2.44}$$

and such that

$$-\frac{1}{2}x^i O_{ij} x^j + J_k x^k = -\frac{1}{2}\bar{x}^i O_{ij} \bar{x}^j + \frac{1}{2}J_k G^{kl} J_l \tag{2.45}$$

Thus, by performing the $d\bar{x}$ integral:

$$I[J] = I[0]\exp\left(\frac{1}{2}J_i G^{ij} J_j\right) \tag{2.46}$$

We can easily transpose that discrete example to our continuum case. Concentrating first on K_E^0 for the sake of clarity (but the discussion on Z^0 will be analogous) we have

$$K_E^0[\beta, J] \;=\; \int \mathscr{D}[x]_E\, e^{-\frac{1}{\hbar}\int\left[\frac{m}{2}x(\tau)\left(-\frac{d^2}{d\tau^2}+\omega^2\right)x(\tau)-J(\tau)x(\tau)\right]}$$

$$=\; \int \mathscr{D}[x]_E\, e^{-\frac{1}{\hbar}\int\left[\frac{1}{2}x(\tau)\hat{O}x(\tau)-J(\tau)x(\tau)\right]}. \tag{2.47}$$

Notice that on the space of functions that vanish at the boundaries (that is at $\tau = \pm\beta/2$) the differential operator $\hat{O} = m(-d^2/d\tau^2 + \omega^2)$ is hermitian and positive definite. As a matter of fact, in terms of its matrix elements between time coordinate eigenstates $\psi_{\tau_1}(\tau) \equiv \delta(\tau - \tau_1)$ and $\psi_{\tau_2}(\tau) \equiv \delta(\tau - \tau_2)$

$$O(\tau_1, \tau_2) \equiv \int d\tau \psi_{\tau_1}(\tau)\hat{O}\psi_{\tau_2}(\tau) = m\left(\partial_{\tau_1}\partial_{\tau_2} + \omega^2\right)\delta(\tau_1 - \tau_2)$$

$$= m\left(-\partial_{\tau_1}^2 + \omega^2\right)\delta(\tau_1 - \tau_2) \tag{2.48}$$

using integration by parts and repeatedly using $x(\pm\beta/2) = 0$, we can rewrite the exponent in eq. (2.47) as

$$-\int \frac{1}{2}x(\tau_1)x(\tau_2)O(\tau_1, \tau_2)d\tau_1 d\tau_2 + \int J(\tau_1)x(\tau_1) \tag{2.49}$$

in full analogy with $-\frac{1}{2}x^i O_{ij}x^j + J_i x^i$ in eq. (2.42) We emphasize here that $O(\tau_1, \tau_2)$ is a function (better a distribution) in the two variables τ_1 and τ_2.

Like in the discrete case, it is convenient to rewrite the exponent using the inverse of $\hat{O}$, that is the Green's function satisfying Dirichlet boundary conditions $G_D(\tau_1.\tau_2)$

$$\hat{O}_{\tau_1}G_D(\tau_1, \tau_2) \equiv m\left(-\partial_{\tau_1}^2 + \omega^2\right)G_D(\tau_1, \tau_2) = \delta(\tau_1 - \tau_2) \tag{2.50}$$

$$G_D\left(\pm\frac{\beta}{2}, \tau\right) = G_D\left(\tau, \pm\frac{\beta}{2}\right) = 0. \tag{2.51}$$

$G_D(\tau_1, \tau_2)$ is just the matrix form of $\hat{O}^{-1}$. Using the two equations above one can also check that $O \cdot G_D \equiv \int O(\tau_1, \tau_3)G_D(\tau_3, \tau_2)d\tau_3 = \delta(\tau_1 - \tau_2)$. The solution of eqs. (2.50,2.51) is given by

$$G_D(\tau_1, \tau_2) = \frac{1}{m\omega}\frac{\sinh\left(\omega\left(\frac{\beta}{2} + \tau_<\right)\right)\sinh\left(\omega\left(\frac{\beta}{2} - \tau_>\right)\right)}{\sinh(\omega\beta)} \tag{2.52}$$

where $\tau_> = \max(\tau_1, \tau_2)$ and $\tau_< = \min(\tau_1, \tau_2)$.

Notice the properties:

$$\lim_{\omega \to 0} G_D(\tau_1, \tau_2) = \frac{1}{m}\left(\frac{\beta}{2} - |\tau_1 - \tau_2| - 2\frac{\tau_1\tau_2}{\beta}\right) \tag{2.53}$$

$$\lim_{\beta \to \infty} G_D(\tau_1, \tau_2) = \frac{1}{2m\omega}e^{-\omega|\tau_1 - \tau_2|} \tag{2.54}$$

Shifting the integration variable

$$x(\tau) = \int G_D(\tau, \tau')J(\tau')d\tau' + y(\tau) \equiv G \cdot J + y \tag{2.55}$$

the exponent is rewritten as (we use $\cdot$ to represent the convolution in τ)

$$\frac{1}{2}x \cdot \hat{O} \cdot x + J \cdot x = \frac{1}{2}(y \cdot \hat{O} \cdot y + J \cdot G_D \cdot \hat{O} \cdot G_D \cdot \hat{J} + 2y \cdot J) - (J \cdot y + J \cdot G_D \cdot J)$$

$$= \frac{1}{2}(y \cdot \hat{O} \cdot y - J \cdot G_D \cdot J) \tag{2.56}$$

so that we find

$$K_E^0[\beta, J] = \exp\left(\frac{1}{2\hbar}\int d\tau_1 d\tau_2 J(\tau_1) G_D(\tau_1, \tau_2) J(\tau_2)\right) \int \mathscr{D}[y]_E e^{-\frac{1}{\hbar}S_E^0[y]} \quad (2.57)$$

$$= e^{\frac{1}{2\hbar}J\cdot G_D\cdot J} K_E^0[\beta, 0] = e^{\frac{1}{2\hbar}J\cdot G_D\cdot J}\sqrt{\frac{m\omega}{2\pi\sinh(\omega\beta)}} \quad (2.58)$$

Following precisely the same steps we can compute the partition function $Z^0[\beta, J]$. The only difference is that in this case the functional integral is over the space of periodic functions in the interval $[-\beta/2, \beta/2]$. The inverse of $\hat{O}$ is now given by the Green's function G_P satisfying period boundary conditions: $G_P(\beta/2, \tau) = G_P(-\beta/2, \tau)$, $G_P(\tau, \beta/2) = G_P(\tau, -\beta/2)$. Thus we find

$$Z^0[\beta, J] = e^{\frac{1}{2\hbar}J\cdot G_P\cdot J}\int_{\text{periodic}} \mathscr{D}[y]_E e^{-\frac{1}{\hbar}S_E^0[y]} \quad (2.59)$$

$$= e^{\frac{1}{2\hbar}J\cdot G_P\cdot J} Z^0[\beta, 0] = \frac{e^{\frac{1}{2\hbar}J\cdot G_P\cdot J}}{2\sinh\frac{\beta\omega}{2\hbar}} \quad (2.60)$$

As for G_P one finds

$$G_P(\tau, \tau') = \frac{1}{2m\omega}\frac{\cosh\left[\omega(\frac{\beta}{2} - |\tau - \tau'|)\right]}{\sinh\left[\omega\frac{\beta}{2}\right]} \quad (2.61)$$

Notice that for $\beta \to \infty$ with τ_1 and τ_2 fixed [1] we have

$$\lim_{\beta\to\infty} G_P = \lim_{\beta\to\infty} G_D = \frac{1}{2m\omega}e^{-\omega|\tau_1-\tau_2|} \quad (2.62)$$

showing that for $\beta \to \infty$ the boundary conditions expectedly do not matter.

2.3.5 Free n-point correlators

Applying the results of the previous section to eqs. (2.38) we obtain a useful expression for the n-point correlators in the free case, that is the harmonic oscillator. The crucial remark is that the J independent prefactors $K_E^0[\beta, 0]$ and $Z^0[\beta, 0]$ drop out from the computation and so we simply get

$$\hbar^{\frac{n}{2}} G_{D,P}(\tau_1, \ldots, \tau_n) = \hbar^{\frac{n}{2}}\left(\prod_{k=1}^{k=n}\frac{\delta}{\delta J(\tau_k)}\right) e^{\frac{1}{2\hbar}J\cdot G_{D,P}\cdot J}\bigg|_{J=0}. \quad (2.63)$$

Notice that via the rescaling $J \to J/\sqrt{\hbar}$ we have put in evidence a factor $\hbar^{\frac{n}{2}}$. As the formulae are the same for Dirichlet and period boundary conditions, we shall drop the P and D in what follows. Working out eq. (2.63) explicitly we find

- for n odd: $G(\tau_1, \ldots, \tau_n) = 0$. This simply follows because $\exp(\frac{1}{2}J \cdot G \cdot J)$ is an even functional of J and we take the limit $J \to 0$ after computing the derivatives.

---

[1] More precisely for $|\tau_1 - \tau_2| \ll \beta$, as well as $|\tau_{1,2} \pm \beta/2| \ll \beta$ for G_D.

- for n even

$$G(\tau_1, \ldots, \tau_n) = \sum_{p \in \sigma_n} G(\tau_{p(1)}, \tau_{p(2)}) \cdots G(\tau_{p(n-1)}, \tau_{p(n)}). \qquad (2.64)$$

σ_n is the group of all permutations of n elements where the permutations differing by the exchange of two elements in a pair or the exchange of a pair are identified. This group contains $\frac{n!}{(n/2)! 2^{(n/2)}} \equiv (n-1)!! = (n-1)(n-3) \cdots 3 \cdot 1$ elements.

Let us see how this works in the simplest cases.

Notice first of all that the two point correlator (D or P) simply equals the corresponding Green's function (thus our notation was wisely chosen!)

$$G(\tau_1, \tau_2) = \frac{\delta}{\delta J(\tau_1)} \frac{\delta}{\delta J(\tau_2)} e^{\frac{1}{2\hbar} J \cdot G_{D,P} \cdot J} \bigg|_{J=0} \qquad (2.65)$$

$$= \frac{\delta}{\delta J(\tau_1)} \int J(\tau) G(\tau, \tau_2) d\tau \, e^{\frac{1}{2\hbar} J \cdot G_{D,P} \cdot J} \bigg|_{J=0} \qquad (2.66)$$

$$= G(\tau_1, \tau_2) \qquad (2.67)$$

To compute the correlator for higher n it is convenient to introduce the graphical notation

A) $\int G(\tau_1, \tau_n) J(\tau_n) d\tau_n \equiv$

B) $G(\tau_1, \tau_2) \qquad \equiv$

Each functional derivative acts in two possible ways:

- on the exponent, i.e. giving a factor like in A)

- on a factor of type A) brought down by a previous derivative, thus giving a factor like in B)

Using the above graphical rules to perform the derivatives one easily sees that after setting $J \to 0$ the terms that survive give eq. (2.64). For instance, the four points correlator is given by the graph shown in figure 2.3

$$G(\tau_1, \tau_2, \tau_3, \tau_4) = G(\tau_1, \tau_2) G(\tau_3, \tau_4) + G(\tau_1, \tau_3) G(\tau_2, \tau_4) +$$
$$G(\tau_1, \tau_4) G(\tau_2, \tau_3). \quad (2.68)$$

The general result we have found is known in quantum field theory as Wick's theorem. It is normally derived by using creation and destruction operators. The path integral allows for a more direct, functional, derivation, which is what we have just shown.
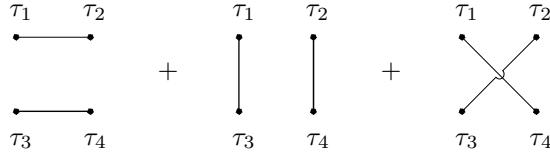
Figure 2.3: A graphical representation of the four points correlator.

2.3.6 The anharmonic oscillator and Feynman diagrams

Using the diagrammatic method outlined in the previous section, and working in a perturbative expansion in ΔV, we can compute the n-point correlators, the propagator and partition function as written in section 2.3.3. For illustrative purposes, we shall focus on the simple example of the anharmonic oscillator with an x^4 potential: $\Delta V = \frac{\lambda_4}{4!} x^4$. We shall compute the leading $O(\lambda_4)$ correction to the free energy. Additional examples, involving other perturbations and other observables, are extensively discussed in the exercise sessions.

From statistical mechanics we have that the free energy $F(\beta)$ of a system in equilibrium at finite temperature is

$$F(\beta) = -\frac{\hbar}{\beta} \ln Z[\beta] \qquad \leftrightarrow \qquad Z[\beta] = e^{-\frac{\beta}{\hbar} F(\beta)} \tag{2.69}$$

We also recall that for $\beta \to \infty$ the partition function is dominated by the ground state, so that in this limit the free energy coincides with the ground state energy

$$\lim_{\beta \to \infty} F(\beta) = E_0 \tag{2.70}$$

Expanding eq. (2.41) at first order in λ_4 we have (notice that we also rescaled $J \to \sqrt{\hbar} J$)

$$Z[\beta] = Z^0[\beta] e^{-\frac{\hbar \lambda_4}{\hbar 4!} \int d\tau \left(\frac{\delta}{\delta J(\tau)} \right)^4} e^{\frac{1}{2} J \cdot G_P \cdot J} \Big|_{J=0} \tag{2.71}$$

$$= Z^0[\beta] \left[1 - \frac{\hbar \lambda_4}{4!} \int d\tau \left(\frac{\delta}{\delta J(\tau)} \right)^4 + \mathcal{O}\left(\lambda_4^2 \right) \right] e^{\frac{1}{2} J \cdot G_P \cdot J} \Big|_{J=0} \tag{2.72}$$

We learned from Wick's theorem that the free four points correlator factorizes as

$$\frac{\delta}{\delta J(\tau_1)} \cdots \frac{\delta}{\delta J(\tau_4)} e^{\frac{1}{2} J \cdot G \cdot J} = (G(\tau_1, \tau_2) G(\tau_3, \tau_4) +$$

$$G(\tau_1, \tau_3) G(\tau_2, \tau_4) + G(\tau_1, \tau_4) G(\tau_2, \tau_3)) \tag{2.73}$$

And thus, in the case at hand, the linear term in the expansion of $Z[\beta]$ is

$$-\frac{\hbar \lambda_4}{4!} \int d\tau \left(\frac{\delta}{\delta J(\tau)} \right)^4 e^{\frac{1}{2} J \cdot G_P \cdot J} \Big|_{J=0} = -\frac{3 \hbar \lambda_4}{4!} \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} G_P^2(\tau, \tau) d\tau \,. \tag{2.74}$$

This result is graphically represented by figure 2.4: it simply corresponds to figure 2.3 in the limiting case in which the four points are taken to coincide,

$\tau_1 = \tau_2 = \tau_3 = \tau_4 = \tau$. The coordinate τ is called the interaction point, and the four lines associated to this point form what is called an interaction vertex. Notice that the factor 3 precisely counts the number of diagrams in the Wick expansion of $G(\tau_1, \tau_2, \tau_3, \tau_4)$. This graphical representation of a term in the perturbative expansion of $Z[\beta]$ is called a Feynman diagram.

$$3G(\tau, \tau)^2 \equiv \quad \tau$$

Figure 2.4: A graphical representation of the part of the propagator linear in λ_4.

Substituting in eq. (2.72) the explicit expression for G_P and performing the (trivial) integral we find

$$Z[\beta] = Z^0[\beta] \left[1 - \frac{\hbar\lambda_4}{32m^2\omega^3}(\omega\beta)\coth^2(\frac{\omega\beta}{2}) + \mathcal{O}\left(\lambda_4^2\right) \right] \qquad (2.75)$$

so that the free energy is

$$F = \frac{\hbar\omega}{2}\left(1 + \frac{1}{\omega\beta}\ln(1 - e^{-\omega\beta}) + \frac{\hbar\lambda_4}{32m^2\omega^3}\coth^2(\frac{\omega\beta}{2}) + \mathcal{O}\left(\lambda_4^2\right) \right) . \qquad (2.76)$$

Notice that the second term in the expression in brackets represents the thermal contribution to the harmonic oscillator free energy, while the third term gives the leading anharmonicity correction. By taking the limit $\beta \to \infty$ we obtain the zero point energy of the anharmonic oscillator at lowest order in λ_4

$$E_0 = \frac{\hbar\omega}{2}\left(1 + \frac{\hbar\lambda_4}{32m^2\omega^3} + \mathcal{O}\left(\lambda_4^2\right) \right) . \qquad (2.77)$$

Some comments on the above results are in order. By eq. (2.77), the dimensionless parameter controlling the perturbative expansion is

$$\bar{\lambda} = \frac{\hbar\lambda_4}{m^2\omega^3} . \qquad (2.78)$$

This result could have been anticipated in various ways. By eq. (2.71) the expansion parameter must be proportional to $\hbar\lambda_4$, which however has dimension mass^2/time^3. With the parameters at hand in the harmonic oscillator, $\bar{\lambda}$ is the only dimensionless parameter proportional to $\hbar\lambda_4$. Also, more directly: the wave function of the harmonic oscillator ground state is localized within a distance $X = \sqrt{\langle x^2 \rangle} \sim \sqrt{\hbar/m\omega}$, and within this distance $\lambda_4 X^4/(m\omega^2 X^2) \sim \bar{\lambda}$, sets the relative size of the perturbation.

While $\bar{\lambda} \ll 1$ is, as was to be expected, necessary to apply perturbation theory, the steps that lead to eqs. (2.76,2.77) leave something to be desired. This is because in eq. (2.75) the first term in the expansion is $\sim \bar{\lambda}\omega\beta$, and becomes infinite in the limit $\beta \to \infty$, suggesting that the higher order terms in the expansion also blow up in this limit. How can we then make sense of our truncation at lowest order? Our procedure to compute E_0 makes sense as long as there exists a range of β where

1. $\sim \bar{\lambda}\omega\beta \ll 1$

2. the contribution of the excited states to $Z(\beta)$ is negligible, that is for

$$e^{-\frac{\beta}{\hbar}(E_1-E_0)} \ll 1 \qquad \longrightarrow \qquad \frac{\beta}{\hbar}(E_1-E_0) \gg 1 \qquad (2.79)$$

which in our case, at lowest order corresponds, to $\omega\beta \gg 1$

The simultaneous satisfaction of 1) and 2) implies again $\bar{\lambda} \ll 1$, and thus our manipulations were technically justified.

But there is more. As a matter of fact, the Hamiltonian formulation tells us that for $\beta \to \infty$ the exact partition function is

$$Z[\beta] \quad \overset{\beta\to\infty}{\longrightarrow} \quad e^{-\frac{\beta}{\hbar}E_0} = e^{-\frac{\beta\omega}{2}\left(1+\frac{\bar{\lambda}}{32}+\cdots\right)} \qquad (2.80)$$

implying that the higher order corrections proportional to $\bar{\lambda}\omega\beta$ in eq. (2.75) must build up into the exponential function. In the technical jargon one says that they must *exponentiate*. Thus even though eq. (2.75) is not a good approximation for $\beta \to \infty$, the structure of the growing terms is fixed to give an exponential. As a corollary $-\ln Z[\beta]/\beta$ is well behaved for $\beta \to \infty$ and for this quantity we can safely apply perturbation theory.

In view of the above discussion we are now motivated to develop a picture on the structure of the higher order terms in the expansion of $Z[\beta]$. The study of the $O(\bar{\lambda}^2)$ contribution is already very suggestive of what happens. Let us focus on it first. Expanding the exponent in eq. (2.71), we find at $O(\lambda_4^2)$

$$\frac{1}{2!}\left(\frac{\hbar\lambda_4}{4!}\right)^2 \int d\tau_1 d\tau_2 \left(\frac{\delta}{\delta J(\tau_1)}\right)^4 \left(\frac{\delta}{\delta J(\tau_2)}\right)^4 e^{\frac{1}{2}J\cdot G_P\cdot J}\bigg|_{J=0} \sim \left\langle x^4(\tau_1)x^4(\tau_2)\right\rangle \tag{2.81}$$

Thus, we have to sum over diagrams that contain two points, τ_1 and τ_2, with four lines ending at each point. We can write three different diagrams, as can be seen in figure 2.5.
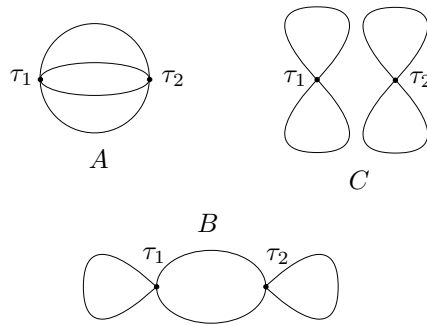

Figure 2.5: The three different diagrams contributing to the corrections to the first energy level of the anharmonic oscillator. Diagrams A and B (at the top-left corner and at the bottom) are connected, while diagram C consists of two disconnected pieces.

The second order term is then shown, by direct computation, to be equal to:

$$\frac{1}{2!}\left(-\frac{\hbar\lambda_4}{4!}\right)^2\int d\tau_1 d\tau_2 \big[24G_P^4(\tau_1,\tau_2)+$$

$$72G_P(\tau_1,\tau_1)G_P^2(\tau_1,\tau_2)G_P(\tau_2,\tau_2) + 9G_P^2(\tau_1,\tau_1)G_P^2(\tau_2,\tau_2)\big] \quad (2.82)$$

where each of these three addenda corresponds to one of the diagrams in figure 2.5.

The numerical factors in front of each of the three factors represents the multiplicity of the corresponding Feynman diagram. It is a useful exercise to reproduce these numbers. Let us do it for diagram A. To count its multiplicity we have to count all possible ways to connect the 4 lines coming out of the τ_1 vertex with the 4 lines coming out of the τ_2 vertex. Let us pick one given line from τ_1: it can connect to τ_2 in **4** possible ways. After having connected this first line, let us pick one of the remaining 3 lines from τ_1: it can connect to τ_2 in **3** possible ways. After this we pick one of the remaining two lines, which can connect to τ_2 in **2** possible ways. The remaining line can connect in just **1** way. Therefore the number of combinations is $4 \times 3 \times 2 \times 1 = 24$. In the same way one can reproduce the factors 72 and 9 associated respectively to diagram B and C. The total number of diagrams is therefore $24+72+9 = 105$. On the other hand, eq. (2.81) tells us that the number of diagrams should be the same as for the correlator among 8 x's (more precisely $\langle x(\tau_1)x(\tau_1)x(\tau_1)x(\tau_1)x(\tau_2)x(\tau_2)x(\tau_2)x(\tau_2)\rangle$). Indeed the combinatoric factor of section 2.3.5 for the 8-point correlator gives $8!/(4!\,2^4) = 105$.

In diagrams A and B there exist at least one line (in fact more) connecting τ_1 and τ_2. These diagrams are therefore called *connected*. On the other hand in diagram C no line exists connecting τ_1 and τ_2: diagram C consists of two *disconnected* copies of the lowest order diagram in Fig.2.4. This implies that the two-dimensional integral corresponding to C factorizes into the square of one-dimensional integral. Diagrams A and B correspond to genuine, non-trivial, two-dimensional integrals.

Putting together the diagrams in Figs. 2.4 and 2.5 the partition function expanded at second order can be written as

$$Z[\beta] = Z_0[\beta]\left[1 - \left(\frac{\hbar\lambda_4}{8}\int G_P^2(\tau,\tau)d\tau\right) + \frac{1}{2}\left(\frac{\hbar\lambda_4}{8}\int G_P^2(\tau,\tau)d\tau\right)^2 + A + B + O(\lambda_4^3)\right]$$

$$(2.83)$$

where we do not have written the explicit expressions of the connected diagrams A and B. The point of the above expression is that the disconnected diagram C has the right coefficient to provide the first step in the exponentiation of the contribution of order λ_4. This pattern continues at higher orders and for all diagrams: the disconnected diagrams just serve the purpose of *exponentiating* the contribution of the connected ones

$$Z[\beta] = Z_0[\beta]\, e^{(\sum \text{connected diagrams})}. \qquad (2.84)$$

For instance, at $O(\lambda_4^3)$, in addition to new connected diagrams, there will be disconnected diagrams corresponding to three copies of Fig. 2.4 and also diagrams made of one copy of Fig. 2.4 with one copy of A (or B). Notice, as it should be evident, that the connected diagrams appear in the above exponent

precisely with the same coefficient they have when they appear for the first time in the expansion of $Z[\beta]$.

The exponentiation in $Z[\beta]$ implies that for the free energy we simply have

$$F = F_0 + \left(\sum \text{connected diagrams} \right) . \tag{2.85}$$

Important result: in order to compute the free energy, and thus also the ground state energy, we only need to compute the connected diagrams.

One can easily check exponentiation of the $O(\lambda_4)$ correction in Fig. 2.4

$$\exp \left(-\frac{\hbar \lambda_4}{4!} \int d\tau \left(\frac{\delta}{\delta J(\tau)} \right)^4 \right) e^{\frac{1}{2} J \cdot G_P \cdot J} \Bigg|_{J=0} =$$

$$\sum_n \frac{1}{n!} \left(-\frac{\hbar \lambda_4}{4!} \right)^n \int d\tau_1 \cdots d\tau_n \left(\frac{\delta}{\delta J(\tau_1)} \right)^4 \cdots \left(\frac{\delta}{\delta J(\tau_n)} \right)^4 \exp \left(\frac{1}{2} J \cdot G_P \cdot J \right) =$$

$$\sum_n \frac{1}{n!} \left[\left(-\frac{3\hbar \lambda_4}{\hbar 4!} \int d\tau G_P^2(\tau, \tau) \right)^n + \text{(other topologies)} \right] =$$

$$\exp \left(-\frac{3\hbar \lambda_4}{4!} \int d\tau G_P^2(\tau, \tau) \right) [1 + \text{(other topologies)}] \tag{2.86}$$

The general proof of eq. (2.84) is an exercise in combinatorics. We shall not present it, but leave it as a challenge to the student. Instead in what follows we want to give a simple proof, valid strictly speaking only for $\beta \to \infty$. It is a refinement of the discussion around eq. (2.80).

Notice first of all that connected diagrams like in figure 2.6 give a contribution that grows linearly in β.
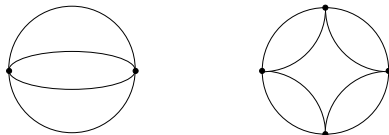

Figure 2.6: Two examples of connected diagrams that contribute to the propagator of the anharmonic oscillator. For example, the diagram on the left corresponds to $\int d\tau_1 d\tau_2 G^4(\tau_1, \tau_2) \sim \beta$.

To prove that, notice that in the large β limit, $G(\tau_1, \tau_2)$ tends to zero exponentially when $\tau_1 \gg \tau_2$. Consider then the general structure of a diagram involving n interaction points

$$\propto \lambda_4^n \int d\tau_1 \ldots d\tau_n F(\tau_1, \ldots, \tau_n) \tag{2.87}$$

where F consists of a product of $G(\tau_i, \tau_j)$. It is graphically obvious that, if a diagram is connected, the associated function F is significantly different than zero only in the region $\tau_1 \simeq \tau_2 \simeq \cdots \simeq \tau_n$ where all time coordinates τ_j are comparable. By integrating first on $\tau_2, \ldots \tau_n$, the integral converges fast and we just get a number c so that

$$\int d\tau_1 d\tau_2 \ldots d\tau_n F(\tau_1, \ldots, \tau_n) = \int d\tau_1 \times c = c\beta \tag{2.88}$$

therefore connected diagrams give a contribution linear in β. This argument easily generalizes to diagrams that consist of 2 or more disconnected pieces. In that case the integrand is non vanishing when the time coordinates are comparable within each connected subdiagram. Therefore a diagram consisting of k disconnected diagrams will produce a contribution growing like β^k.

Thus for $\beta \to \infty$ we have

$$Z[\beta] = Z_0[\beta] \left(1 + A_1\beta + A_2\beta^2 + \dots \right) \tag{2.89}$$

where A_k is a sum over all diagrams involving k connected subdiagrams. In particular A_1 is the sum over the connected diagrams.

Now, since $Z[\beta] \sim e^{-\beta E_0}$, the coefficients of β^n must be such as to exponentiate $A_1\beta$, i.e.

$$A_n = \frac{1}{n!}(A_1)^n \tag{2.90}$$

and we can write:

$$\lim_{\beta \to \infty} Z[\beta] = \lim_{\beta \to \infty} Z_0[\beta]e^{A_1\beta} \tag{2.91}$$

$$\Rightarrow E_0 = \frac{\hbar\omega}{2} - \hbar A_1$$

Once again we found that the ground state energy is given by the sum of all connected diagrams.

Chapter 3

The semiclassical approximation

Let us ask an intuitive question. When do we expect the wave nature of a particle propagation to be well appoximated by the properties of the trajectory of a classical particle?

Well, as for the propagation of light, when the wavelength λ is much smaller than the characteristic physical size of the system, diffraction phenomena are unimportant, and we can use geometric optics.

In the quantum case, we expect similar results: if the wavelength λ is short enough with respect to the typical length over which the potential varies L, we can expect to be able to form a wave packet of size between λ and L, whose motion should be well appoximated by that of a classical particle.

We have two approximation methods to analytically treat systems that cannot be solved exactly:

Perturbation theory: Let us assume we are dealing with a system whose hamiltonian H can be written as $H = H_0 + \lambda H_p$ where H_0 is exactly solvable and λH_p can be treated as a small perturbation (that is $|\lambda \langle n|H_p|m\rangle| \ll |E_n^{(0)} - E_m^{(0)}|$, where $|n\rangle$ and $E_n^{(0)}$ are respectively the eigenstates and eigenvalues of H_0). In this case, we work in perturbation theory in λ and we compute the eigenvalues of the hamiltonian E_n as a series in λ:

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

and similarly we expand the eigenvectors H.

Semiclassical methods: We use these methods when a system is close to the classical limit $\hbar \to 0$, but more generally also when dealing with tunneling phenomena. These methods offer no diagrammatic representation: when small couplings are involved, semiclassical contributions are proportional to e^{-1/λ^2} and thus they offer non-perturbative corrections to the system.

3.1   The semiclassical propagator

The goal of this section is to compute the leading contribution to the path integral in the formal limit $\hbar \to 0$. In practice this will correspond to deriving a general expression for the Gaussian, or semiclassical, approximation discussed in section 1.3.2. Let us recall it. Starting from the propagator

$$K(x_f, t_f; x_i, t_i) = \int \mathscr{D}[x] e^{i \frac{S[x]}{\hbar}} \tag{3.1}$$

we expand it around the classical solution x_c: $x = x_c + y$ and get

$$K(x_f, t_f; x_i, t_i) = e^{i \frac{S[x_c]}{\hbar}} \int \mathscr{D}[y] e^{\frac{i}{\hbar}\left(\frac{1}{2}\frac{\delta^2 S}{\delta x^2} y^2 + \frac{1}{3!}\frac{\delta^3 S}{\delta x^3} y^3 + \cdots\right)} \tag{3.2}$$

The rescaling $y = \sqrt{\hbar}\tilde{y}$ makes it evident that the expansion in powers of y truly corresponds to an expansion in powers of $\hbar$

$$K(x_f, t_f; x_i, t_i) = \mathcal{N} \cdot e^{i \frac{S[x_c]}{\hbar}} \int \mathscr{D}[\tilde{y}] e^{\frac{i}{2}\frac{\delta^2 S}{\delta x^2}\tilde{y}^2 + \sqrt{\hbar}\mathcal{O}(y^3)}. \tag{3.3}$$

Finally, dropping orders higher than the second in the Taylor expansion of the action, we obtain the Gaussian, or semiclassical, approximation to the propagator:

$$K_{sc}(x_f, t_f; x_i, t_i) = \mathcal{N} \cdot e^{i \frac{S[x_c]}{\hbar}} \int \mathscr{D}[\tilde{y}] e^{\frac{i}{2}\frac{\delta^2 S}{\delta x^2}\tilde{y}^2} \tag{3.4}$$

Let us now consider the simple case where:

$$S[x] = \int \left(\frac{m\dot{x}^2}{2} - V(x)\right) dt \tag{3.5}$$

We can expand at quadratic order around x_c:

$$\frac{m\dot{x}^2}{2} \to \frac{m\dot{\tilde{y}}^2}{2}$$
$$V(x) \to \frac{1}{2}V''(x_c)\tilde{y}^2$$

where we used the notation $V''(x_c) = \partial_x{}^2 V(x)|_{x=x_c}$.

Thus, we must compute:

$$I[x_c] = \mathcal{N} \int \mathscr{D}[\tilde{y}] e^{\frac{i}{2}\int dt \left(m\dot{\tilde{y}}^2 - V''(x_c)\tilde{y}^2\right)}. \tag{3.6}$$

This is a Gaussian path integral like the one we found for the harmonic oscillator in subsection 1.3.4. More precisely if we write $V''(x_c(t)) \equiv \Omega^2(t)$, the computation generalizes that of the fluctuation determinant for the harmonic oscillator, for which $\Omega^2(t) = \omega^2$ is time independent. We can thus proceed along the same lines of subsection 1.3.4 and first perform the change of variables

$$\tilde{y}(t) = \sum_n \tilde{a}_n y_n(t) \tag{3.7}$$

where y_n are the orthonormalized eigenmodes of the differential operator

$$\left[-m\frac{d^2}{dt^2} - V''(x_c(t))\right] \equiv \left[-m\frac{d^2}{dt^2} - \Omega^2(t)\right] \tag{3.8}$$

which controls the quadratic action. We have again the change of measure[1]

$$\mathcal{N} \cdot \mathscr{D}[\tilde{y}(t)] = \tilde{\mathcal{N}} \cdot \prod_n \frac{d\tilde{a}_n}{\sqrt{2\pi i}} \tag{3.9}$$

so that in the end the gaussian integral in eq. (3.6) gives

$$I[x_c] = \tilde{\mathcal{N}}\left(\det\left(-m\frac{d^2}{dt^2} - V''(x_c)\right)\right)^{-\frac{1}{2}} = \tilde{\mathcal{N}}D^{-\frac{1}{2}} \tag{3.10}$$

One final, important, remark before going to the computation, is that the Jacobian factor $\tilde{\mathcal{N}}$ is independent of $V''(x_c(t))$. Consider indeed choosing a different orthonormal basis $\{y_n'(t)\}$ on the space of square integrable functions on the time interval $T = t_f - t_i$

$$\tilde{y}(t) = \sum_n \tilde{a}_n y_n(t) = \sum_m \tilde{a}_m' y_m'(t) . \tag{3.11}$$

We have

$$\tilde{a}_n = U_{nm}\tilde{a}_m' \tag{3.12}$$

where U_{mn} is an (infinite) unitary matrix satisfying $U^\dagger U = \mathbb{1}$ and $\det U = 1$ as it follows from standard linear algebra given that the two sets $\{y_n(t)\}$, $\{y_n'(t)\}$ are orthonormalized. We thus have

$$\prod_n \frac{d\tilde{a}_n}{\sqrt{2\pi i}} = \prod_m \frac{d\tilde{a}_m'}{\sqrt{2\pi i}} \tag{3.13}$$

which proves that the Jacobian $\tilde{\mathcal{N}}$ is independent of the orthonormal basis and, a fortiori, is independent of whatever differential operator has that basis as its eigenbasis.

Let us now proceed. The computation of determinants as in eq. (3.10) was first carried out by Gelfand and Yaglom. In our derivation we shall follow a clever, but less formal, derivation due to Coleman. A more mathematical derivation can be found in [8]. The result we are are going to prove is that

$$\frac{D}{\tilde{\mathcal{N}}^2} = c \cdot \psi_0(t_f) \tag{3.14}$$

where:

- $\psi_0(t)$ satisfies the differential equation

$$-\left(\frac{md^2}{dt^2} + \Omega^2(t)\right)\psi_0(t) = 0 \tag{3.15}$$

  with the boundary conditions

$$\psi_0(t_i) = 0 \qquad \psi_0'(t_i) = 1 . \tag{3.16}$$

---

[1]Notice that, just to confuse the reader(!), we use a different simbol for the Jacobian with respect to eq. (1.90). This is because we are now working with rescaled variables $\tilde{y}$ and $\tilde{a}_n$ which absorbed a power of $\hbar$. This is to orient the reader on the origin of the factors, but beware that these Jacobians are anyway ill defined when $\epsilon \to 0$!

- c is a constant that does not depend on $\Omega^2(t)$, and thus we can compute it in the free particle case, $\Omega^2(t) = 0$.

Consider now two different time dependent frequencies: $\Omega_1^2(t)$ and $\Omega_2^2(t)$. Consider also the solution of the "eigenvalue" equation, generalizing eq. (3.15):

$$\underbrace{-\left(\frac{md^2}{dt^2} + \Omega_1^2(t)\right)\psi_\lambda^{(1)}(t)}_{\hat{O}_1} = \lambda\psi_\lambda^{(1)}(t) \tag{3.17}$$

with boundary conditions

$$\psi_\lambda^{(1)}(t_i) = 0 \qquad \partial_t\psi_\lambda^{(1)}(t_i) = 1 \,. \tag{3.18}$$

- For all λ, these two conditions fix the solution everywhere, and thus we can compute $\psi_\lambda^{(1)}(t_f)$.

- λ is an eigenvalue of $\hat{O}_1$ if, and only if $\psi_\lambda^{(1)}(t_f) = 0$. Indeed, remember that we are looking for the eigenvalues of $\hat{O}_1$ over the space of functions that vanish at t_i and t_f.

Consider then the same problem for $\hat{O}_2 \equiv -\left(\frac{md^2}{dt^2} + \Omega_2^2(t)\right)$ and call $\psi_\lambda^{(2)}$ the solution of the differential equation $\hat{O}_2\psi_\lambda^{(2)} = \lambda\psi_\lambda^{(2)}$ with the same boundary conditions in 3.18.
We have then the following

Theorem:

$$\frac{\det\left(\hat{O}_1 - \lambda\right)}{\det\left(\hat{O}_2 - \lambda\right)} = \frac{\psi_\lambda^{(1)}(t_f)}{\psi_\lambda^{(2)}(t_f)} \tag{3.19}$$

We shall now prove the above by following Coleman, and, as it is customary in physics, emphasizing ideas above mathematical rigour.
Let us define first:

$$f(\lambda) = \frac{\psi_\lambda^{(1)}(t_f)}{\psi_\lambda^{(2)}(t_f)} \tag{3.20}$$

f satisfies the following properties:

- $f(\lambda)$ has obviously all its zeroes in correspondence with the eigenvalues of $\hat{O}_1$ and all its poles in correspondence with eigenvalues of $\hat{O}_2$. All these zeroes and poles are *simple* as we show in the mathematical appendix of subsection 3.1.2.

- $f(\lambda) \to 1$ in the limit $\lambda \to \infty$, $\lambda \notin \mathbb{R}_+$. This property follows by simple solution of the differential equation 3.17. Indeed, for $\lambda \to \infty$, we can neglect $\Omega_{1,2}^2(t)$, and thus the solution satisfying the boundary conditions 3.18 is written as (see the mathematical appendix 3.1.3 for more detail)

$$\psi_\lambda^{(1,2)}(t) = \frac{1}{2i}\sqrt{\frac{m}{\lambda}}\left(e^{i\sqrt{\frac{\lambda}{m}}(t-t_i)} - e^{-i\sqrt{\frac{\lambda}{m}}(t-t_i)}\right) + \mathcal{O}\left(\frac{\Omega_{1,2}^2}{\lambda}\right) \tag{3.21}$$

One of the two exponentials grows for $\lambda \notin \mathbb{R}_+$. Thus, there are no zeroes at $t = t_f$, and we can safely neglect $\Omega_{1,2}^2$ for all t. On the other hand, for $\lambda/m = [n\pi/(t_f - t_i)]^2$, the zeroth order solution (first term in eq. (3.21)) vanishes at $t = t_f$ and therefore the $\Omega_{1,2}^2$ perturbation cannot be treated as small, showing that $\lim_{\lambda \to \infty} f(\lambda) \neq 1$ for $\lambda \in \mathbb{R}_+$.

Consider now:

$$g(\lambda) = \frac{\det\left(\hat{O}_1 - \lambda\right)}{\det\left(\hat{O}_2 - \lambda\right)} = \frac{\det\left(-m\partial_t^2 - \lambda - \Omega_1^2\right)}{\det\left(-m\partial_t^2 - \lambda - \Omega_2^2\right)} \qquad (3.22)$$

- It has exactly the same simple poles and simple zeroes as $f(\lambda)$.

- For $\lambda \to \infty$, $\lambda \notin \mathbb{R}_+$, we have $g(\lambda) \to 1$. Without aiming at mathematical rigour (but a more thorough discussion is presented in Homework 8) this result is qualitatively understood as follows. Notice that $\hat{T} \equiv -m\partial_t^2 - \lambda$ has eigenvalues $\lambda_n = (n\pi/(t_f - t_i))^2 - \lambda$. This result for λ_n implies that the norm $|\lambda_{min}|$ of the eigenvalue of smallest norm λ_{min} goes to infinity when $\lambda \to \infty$, $\lambda \notin \mathbb{R}_+$. In this situation the addition to this operator of Ω_1^2 or Ω_2^2 is a small perturbation with negligible effects as $\lambda \to \infty$. Therefore we expect $g(\lambda) \to 1$ for $\lambda \to \infty$, $\lambda \notin \mathbb{R}_+$. Obviously this reasoning does not work for $\lambda \in \mathbb{R}_+$, as the function g has zero and poles for arbitrarily large λ.

Putting everything together we have that the ratio

$$h(\lambda) = \frac{f(\lambda)}{g(\lambda)}$$

is analytic everywhere (the singularity at the simple poles of f is neutralized by simple zeroes of $1/g$ and conversely the singularity at the simple zeroes of g is neutralized by simple zeroes of f) and tends to 1 as $\lambda \to \infty$. By Cauchy theorem the only such function is $h(\lambda) \equiv 1$, and that proves our theorem. More precisely, applying Cauchy theorem to $h(\lambda) - 1$ and integrating over a circle C with radius $R \to \infty$ we have

$$h(\lambda) - 1 = \frac{1}{2\pi i} \oint_C \frac{h(z) - 1}{z - \lambda} dz \to 0 \qquad (3.23)$$

where in the last step we used that $\lim_{|z| \to \infty}(h(z) - 1) = 0$.

Consider now $\Omega_1^2(t) \equiv \Omega^2(t)$ and call $\psi_0^{(\Omega)}$ the solution to the problem in eqs. (3.17,3.18) at $\lambda = 0$. As a corollary of eq. (3.19) we have that

$$\frac{\det\left(-\frac{md^2}{dt^2} - \Omega^2(t)\right)}{\tilde{\mathcal{N}}^2} \frac{1}{\psi_0^{(\Omega)}(t_f)} = c \qquad (3.24)$$

where c is independent of $\Omega(t)$, and where we have judiciously inserted the normalization Jacobian (which, like c, is independent of Ω^2) in order to deal only with the physically interesting combination $\tilde{\mathcal{N}}/\text{Det}^{1/2}$. Provided we find the

constant c, the solution to the differential equation problem in eqs. (3.17,3.18) at $\lambda = 0$, gives us the determinant we were after! Finding the constant c is easy: we just need to use eq. (3.24) for an operator whose determinat we already know. The easiest option to do so is to consider the free particle case, where $\Omega(t) = 0$. In this case the determinat prefactor in K was computed in eq. (1.48)

$$\frac{1}{\tilde{\mathcal{N}}^2} \det\left(-\frac{md^2}{dt^2}\right) = \frac{2\pi i(t_f - t_i)\hbar}{m} \qquad (3.25)$$

while the solution to eqs. (3.15,3.16) is

$$\psi_0^{(0)}(t) = t - t_i \qquad (3.26)$$

and thus:

$$c = \frac{2\pi i\hbar}{m} \qquad (3.27)$$

The result for the gaussian integral in the general case is then

$$I[x_c] = \sqrt{\frac{m}{2\pi i\hbar\psi_0^{(\Omega)}(t_f)}} \qquad (3.28)$$

3.1.1   VanVleck-Pauli-Morette formula

Let us now derive a useful implicit expression for $\psi_0^{(\Omega)}(t_f)$. The classical equation of motion tells us

$$m\ddot{x}_c + V'(x_c) = 0 \qquad (3.29)$$

where the dot denotes derivation with respect to time. By differentiating it once we get

$$m\dddot{x}_c + V''(x_c)\dot{x}_c = 0 \qquad (3.30)$$

Thus, $v_c = \dot{x}_c$ satisfies the differential equation that we are trying to solve in order to find $\psi_0^{(\Omega)}(t)$. However, it doesn't satisfy in general the boundary conditions $\psi_0(t_i) = 0$, $\partial_t\psi_0(t_i) = 1$. Consider now the Wronskian:

$$W(t) = v_c(t)\dot{\psi}_0(t) - \dot{v}_c(t)\psi_0(t) \qquad (3.31)$$

where $\psi_0(t) = \psi_0^{(\Omega)}(t)$ is the function we are looking for.

Since ψ and v_c satisfy the same differential equation, we have $\dot{W}(t) = 0$, and thus $W(t) = W$ is a constant. We can then write:

$$v_c{}^2 \frac{d}{dt}\left(\frac{\psi_0}{v_c}\right) = v_c{}^2\left(\frac{\dot{\psi}_0}{v_c} - \frac{\psi_0\dot{v}_c}{v_c{}^2}\right) = W = v_c(t_i)$$

$$\Rightarrow \frac{d}{dt}\left(\frac{\psi_0}{v_c}\right) = v_c(t_i)\frac{1}{v_c{}^2}$$

$$\Rightarrow \psi_0(t) = v_c(t)v_c(t_i)\int_{t_i}^{t}\frac{1}{v_c{}^2(t')}dt'$$

$$\Rightarrow \psi_0(t_f) = v_c(t_f)v_c(t_i)\int_{t_i}^{t_f}\frac{1}{v_c{}^2(t')}dt' \qquad (3.32)$$

Let us now write $\psi_0(t_f)$ in terms of energy and potential. We have, from the classical solution: $\frac{mv_c{}^2(t)}{2} = E - V(x_c(t))$, and $dt = \frac{dx}{v_c}$. Writing $v_f = v_c(t_f)$ and $v_i = v_c(t_i)$:

$$\psi_0(t_f) = v_f v_i \int_{x_i}^{x_f} \left(\frac{m}{2(E - V(x))} \right)^{\frac{3}{2}} dx \tag{3.33}$$

$$\equiv v_f v_i \int_{x_i}^{x_f} \frac{dx}{v(x)^3} \tag{3.34}$$

The prefactor is then:

$$I[x_c] = \sqrt{\frac{1}{2\pi i \hbar v_f v_i \sqrt{m} \int_{x_i}^{x_f} \frac{dx}{2(E - V(x))}}} \tag{3.35}$$

Or in terms of velocities:

$$I[x_c] = \sqrt{\frac{m}{2\pi i \hbar v_f v_i \int_{x_i}^{x_f} \frac{dx}{v^3(x)}}} \tag{3.36}$$

Let us now express the result in terms of the classical action. We have:

$$S_c = \int_{t_i}^{t_f} \left(\frac{m\dot{x}_c{}^2}{2} - V \right) dt = \int_{t_i}^{t_f} \left(m\dot{x}_c{}^2 - E \right) dt =$$
$$\int_{x_i}^{x_f} \sqrt{2m(E - V(x))} dx - E(t_f - t_i) \tag{3.37}$$

Thus:

$$\frac{\partial S_c}{\partial x_f} = P_f = \sqrt{2m(E - V(x_f))} \tag{3.38}$$

$$\frac{\partial^2 S_c}{\partial x_i \partial x_f} = \frac{\partial P_f}{\partial x_i} = \frac{1}{2} \sqrt{\frac{2m}{E - V(x_f)}} \frac{\partial E}{\partial x_i} = \frac{1}{v_f} \frac{\partial E}{\partial x_i} \tag{3.39}$$

We can note that:

$$t_f - t_i = \int_{t_i}^{t_f} dt = \int_{x_i}^{x_f} \frac{dx}{\dot{x}} = \int_{x_i}^{x_f} \sqrt{\frac{m}{2(E - V(x))}} dx \tag{3.40}$$

$$0 = \frac{\partial(t_f - t_i)}{\partial x_i} = -\frac{1}{v_i} - \frac{1}{2} \frac{\partial E}{\partial x_i} \int_{x_i}^{x_f} \sqrt{\frac{m}{2}} \frac{dx}{(E - V(x))^{\frac{3}{2}}}$$

$$\Rightarrow \frac{\partial E}{\partial x_i} = -\frac{m}{v_i \int_{x_i}^{x_f} \frac{dx}{v^3(x)}} \tag{3.41}$$

Thus, the derivative of the action can be written as:

$$\frac{\partial^2 S_c}{\partial x_i \partial x_f} = -\frac{m}{v_i v_f \int_{x_i}^{x_f} \frac{dx}{v^3(x)}} \tag{3.42}$$

And we get in the end the Van Vleck-Pauli-Morette determinant:

$$I[x_c] = N \sqrt{\frac{1}{\det \left(-m\frac{d^2}{dt^2} - V''(x_c) \right)}} = \sqrt{-\frac{1}{2\pi i \hbar} \frac{\partial^2 S_c}{\partial x_i \partial x_f}} \tag{3.43}$$

And thus we can write the final form of the semiclassical propagator:

$$K_{sc}(x_f, t_f; x_i, t_i) = e^{i\frac{S_c}{\hbar}} \sqrt{-\frac{1}{2\pi i\hbar} \frac{\partial^2 S_c}{\partial x_i \partial x_f}} \tag{3.44}$$

3.1.2   Mathematical Appendix 1

Let us now prove that $\psi_\lambda(t_f)$ only has simple zeroes. Consider the equation:

$$\left(-\frac{md^2}{dt^2} + V\right)\psi_\lambda(t) = \lambda\psi_\lambda(t) \tag{3.45}$$

with the boundary conditions $\psi_\lambda(t_i) = 0$, $\partial_t\psi_\lambda(t_i) = 1$.

We will use the notation:

$$\dot{\psi}_\lambda(t) \equiv \frac{d}{d\lambda}\psi_\lambda(t)$$

$$\psi'_\lambda(t) \equiv \frac{d}{dt}\psi_\lambda(t)$$

When we differentiate (3.45) with respect to λ, we get:

$$\left(-\frac{md^2}{dt^2} + V\right)\dot{\psi}_\lambda(t) = \lambda\dot{\psi}_\lambda(t) + \psi_\lambda(t) \tag{3.46}$$

Notice that since we impose the same boundary conditions for all λ, we have:

$$\dot{\psi}_\lambda(t_i) = \dot{\psi}'_\lambda(t_i) = 0 \tag{3.47}$$

Consider then the "Wronskian":

$$W = \psi_\lambda\dot{\psi}'_\lambda - \psi'_\lambda\dot{\psi}_\lambda \tag{3.48}$$

$$W' = \psi_\lambda\dot{\psi}''_\lambda - \psi''_\lambda\dot{\psi}_\lambda$$

$$= \psi_\lambda\frac{1}{m}\left[(V-\lambda)\dot{\psi}_\lambda - \psi_\lambda\right] - \frac{1}{m}(V-\lambda)\psi_\lambda\dot{\psi}_\lambda$$

$$= -\frac{\psi_\lambda^2}{m} \leqslant 0 \tag{3.49}$$

On the other hand, we have the boundary conditions:

$$W(t_i) = 0, \qquad W(t_f) = \psi_\lambda(t_f)\dot{\psi}'_\lambda(t_f) - \psi'_\lambda(t_f)\dot{\psi}_\lambda(t_f) \tag{3.50}$$

Thus, if both $\psi_\lambda(t_f)$ and $\dot{\psi}_\lambda(t_f)$ vanish, the Wronskian is zero everywhere, and so is its derivative. Thus, $\psi_\lambda(t) \equiv 0$.

3.1.3   Mathematical Appendix 2

We want to write explicitly the solution to

$$(-\partial_t^2 - \lambda - \Omega^2(t))\psi = 0 \qquad \psi(0) = 0, \quad \psi'(0) = 1 \tag{3.51}$$

treating $\Omega^2(t)$ as a perturbation. In order to carry on perturbation theory in Ω^2 we need the retarded Green's function for the zeroth order equation $G(t, t') =$

$\hat{T}^{-1}$ where $\equiv \hat{T} \equiv -\partial_t^2 + \lambda$. By a simple computation analogous to the one used to find the euclidean Green's function one finds (see section III of ref. [8] for instance)

$$G(t,t') = \theta(t-t')\frac{1}{2i\sqrt{\lambda}}\left(e^{-2i\sqrt{\lambda}(t-t')} - e^{2i\sqrt{\lambda}(t-t')}\right). \qquad (3.52)$$

Also defining the zeroth order solution

$$\psi_0 = \frac{1}{2i\sqrt{\lambda}}\left(e^{i\sqrt{\lambda}(t-t_i)} - e^{-i\sqrt{\lambda}(t-t_i)}\right) \qquad (3.53)$$

and writing $\psi = \psi_0 + \phi$, eq. (3.51) becomes

$$\hat{T}\phi = \Omega^2(\psi_0 + \phi) \qquad (3.54)$$

which by use of $G = \hat{T}^{-1}$ and by employing standard functional operator notation (by $\circ$ we indicate the product of functional operators), can be written as

$$(\mathbb{1} - G \circ \Omega^2)\phi = G \circ \Omega^2 \psi_0 \qquad (3.55)$$

and solved iteratively in ϕ

$$\phi = (\mathbb{1} - G \circ \Omega^2)^{-1} G \circ \Omega^2 \psi_0 = \sum_{n=1}^{\infty}(G \circ \Omega^2)^n \psi_0 \qquad (3.56)$$

and therefore

$$\psi = \sum_{n=0}^{\infty}(G \circ \Omega^2)^n \psi_0. \qquad (3.57)$$

Notice that ψ defined above automatically satisfies the boundary conditions $\psi(0) = 0$, $\psi'(0) = 1$. For the lowest order correction we have

$$(G \circ \Omega^2)\psi_0 = \int_0^t dt' \frac{1}{2i\sqrt{\lambda}}\left(e^{-2i\sqrt{\lambda}(t-t')} - e^{2i\sqrt{\lambda}(t-t')}\right)\Omega^2(t')\psi_0(t') \qquad (3.58)$$

which for $\lambda \notin \mathbb{R}_+$ is $\sim O(\Omega^2/\sqrt{\lambda})\psi_0$.

3.2 The fixed energy propagator

3.2.1 General properties of the fixed energy propagator

The fixed-energy retarded propagator, sometimes simply Green's function, is defined as the Fourier transform of the retarded propagator $\theta(t)K(x_f, t; x_i, 0)$

$$\begin{aligned}
K(E; x_f, x_i) &\equiv \int_0^\infty K(x_f, t; x_i, 0)e^{\frac{iEt}{\hbar}}\, dt \\
&= \int_0^\infty \langle x_f| e^{-\frac{i\hat{H}t}{\hbar} + \frac{iEt}{\hbar}} |x_i\rangle\, dt \\
&= \lim_{\epsilon \to 0} \int_0^\infty \langle x_f| e^{\frac{it}{\hbar}(E - \hat{H} + i\epsilon)} |x_i\rangle\, dt \\
&= \lim_{\epsilon \to 0} \langle x_f| \frac{i\hbar}{E - \hat{H} + i\epsilon} |x_i\rangle \qquad (3.59)
\end{aligned}$$

where, as usual when dealing with distributions, the factor $e^{-\epsilon t/\hbar}$ with $\epsilon \to 0^+$ is introduced to insure converge of the integral at $t \to \infty$. Notice that since we integrate over $t > 0$, the exponent $e^{iEt/\hbar}$ ensures strong convergence of the integral for any E in the upper complex plane, that is for $\mathrm{Im}E > 0$. For $\mathrm{Im}E > 0$ the retarded propagator $K(E; x_f, x_i)$ is thus an analytic function of the complex variable E. This is an important property of retarded Green's functions: analyticity in the upper energy plane is the Fourier space manifestation of causality, that is of retardation. For the advanced propagator we would have instead analyticity in the lower complex E plane.

From the last equation above, the retarded propagator $K(E; x_f, x_i)$ is just the position space representation of the inverse of the Schrödinger operator, $\hat{K} = \frac{i\hbar}{E - \hat{H} + i\epsilon}$. It thus satisfies the relation:

$$\lim_{\epsilon \to 0}(E - \hat{H} + i\epsilon)\hat{K} = i\hbar \mathbb{1} \tag{3.60}$$

In coordinate representation, equation (3.60) becomes:

$$\left(-\frac{\hbar^2}{2m}\partial_x{}^2 + V(x) - E\right)K(E; x, y) = -i\hbar\delta(x - y). \tag{3.61}$$

This equation, and the boundary conditions we discuss below, fully fix $K(E; x_f, x_i)$. Let us discuss this in detail. Given two linearly independent solutions ψ_1 and ψ_2 of the homogeneous Schrödinger's equation at energy E

$$\left(-\frac{\hbar^2}{2m}\partial_x{}^2 + V(x) - E\right)\psi_{1,2} = 0 \tag{3.62}$$

the following function satisfies eq. (3.61)

$$f(E; x, y) = \frac{2mi}{\hbar W}\left(\theta(x - y)\psi_1(x)\psi_2(y) + \theta(y - x)\psi_2(x)\psi_1(y)\right) \tag{3.63}$$

where $W = \psi_1'(x)\psi_2(x) - \psi_2'(x)\psi_1(x)$ is the wronskian; we recall that, by eq. (3.62), W is constant over x. However in order for eq. (3.63) to coincide with the retarded propagator, we must choose ψ_1 and ψ_2 satisfying the appropriate boundary conditions. Which boundary conditions are required? The answer is obtained by simple physical considerations. In order to illustrate that, let us work on a case by case basis.

Let us focus first on motion in a potential $V(x)$ satisfying $\lim_{|x| \to \infty} V(x) = 0$, which is relevant for barrier penetration problems and in the case of potential wells of finite spacial width. In this situation any solution ψ of the Schroedinger equation with positive energy behaves at $|x| \to \infty$ as a linear combination of outgoing and ingoing plane waves

$$\lim_{x \to +\infty} \psi = a_+ e^{-i\sqrt{2mE}x} + b_+ e^{-i\sqrt{2mE}x} \tag{3.64}$$

$$\lim_{x \to -\infty} \psi = a_- e^{-i\sqrt{2mE}x} + b_- e^{-i\sqrt{2mE}x} \tag{3.65}$$

The solutions $\psi_{1,2}$ are selected by requiring $K(E; x_f, x_i)$ to have the physically correct behaviour at $|x_f| \to \infty$. To find out which behaviour is the physically correct one, we must recall that the inverse Fourier transform, the propagator,

$$K(x_f, t; x_i, 0) = \int_{-\infty}^{\infty} K(E; x_f, x_i)e^{-iEt/\hbar}\frac{dE}{2\pi\hbar} \tag{3.66}$$

represents the wave function $\Psi(x_f, t)$ at $t > 0$ for a state which at $t = 0$ was a δ-function at some finite position x_i, that is $\lim_{t \to 0} \Psi(x_f, t) = \delta(x_f - x_i)$. Then at any finite $t > 0$, for $x_f \to +\infty \gg x_i$, the wave function $\Psi(x_f, t)$ should correspond to a superposition of waves travelling out in the positive x direction, ie with positive momentum and positive energy. This implies

$$\lim_{x_f \to +\infty} K(E; x_f, x_i) \propto e^{+i\sqrt{2mE}x_f} \tag{3.67}$$

Similarly, for $x_f \to -\infty$, $\Psi(x_f, t)$ should be a superposition of waves travelling out in the negative x direction, ie with negative momentum

$$\lim_{x_f \to -\infty} K(E; x_f, x_i) \propto e^{-i\sqrt{2mE}x_f} \tag{3.68}$$

This gives us all the constraints to fully fix $\psi_{1,2}$ and write a general expression for $K(E; x_f, x_i)$ in the form 3.63. Before discussing that, notice that, analiticity in the upper energy plane, tells us to how to continue $\sqrt{E}$ from $E > 0$ to $E < 0$ [2]. Then for $E < 0$ (or more precisely $E = \lim \epsilon \to 0^+(-|E| + i\epsilon)$ the above asymptotic behaviours become

$$\lim_{x_f \to +\infty} K(E; x_f, x_i) \quad \propto \quad e^{-\sqrt{2m|E|}x_f} \to 0 \tag{3.69}$$

$$\lim_{x_f \to -\infty} K(E; x_f, x_i) \quad \propto \quad e^{+\sqrt{2m|E|}x_f} \to 0 \tag{3.70}$$

corresponding to K representing an operator on the space of normalizable wave functions. Indeed to find the correct boundary conditions we could have worked the other way around, and consider first the asymptotic behaviour of $K(E, x_f, x_i)$ for $E < 0$. By eq. (3.61) there are two possibilities: $e^{+\sqrt{2m|E|}x_f}$ and $e^{-\sqrt{2m|E|}x_f}$. The request that K be square integrable implies the choice in eqs. (3.69, 3.70). Then by analytically continuing eqs. (3.69, 3.70) to $E > 0$ through a path in the Im $E > 0$ half-plane we get the outgoing wave boundary conditions of eqs. (3.67, 3.68). [3]

By eq. (3.63) the behaviour at $x_f \to +\infty$ and $x_f \to -\infty$ is controlled respectively by ψ_1 and ψ_2. Then eqs. (3.67, 3.68) are satisfied if

$$\lim_{x \to +\infty} \psi_1(x) \quad \propto \quad e^{+i\sqrt{2m|E|}x} \tag{3.71}$$

$$\lim_{x \to -\infty} \psi_2(x) \quad \propto \quad e^{-i\sqrt{2m|E|}x} \tag{3.72}$$

and provided we have such two solutions we can write the retarded propagator as

$$K(E; x, y) = \frac{2mi}{\hbar W} \left(\theta(x - y)\psi_1(x)\psi_2(y) + \theta(y - x)\psi_2(x)\psi_1(y) \right) \tag{3.73}$$

Summarizing: retardation corresponds to outgoing waves at $x \to \pm\infty$.

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[2]This is because the cut of $\sqrt{E}$ should be chosen at Im $E < 0$ to ensure analyticity of $K(E; x_f, x_i)$ at Im $E > 0$.

[3]On the other hand, if we continue eq. (3.70) to $E > 0$ by a path in the Im $E < 0$ half-plane we would get incoming instead of outgoing boundary conditions. This would correspond to the advanced propagator, which is analytic in the lower energy half-plane.

We can generalize these considerations to other potentials. For instance consider the case where $\lim_{x \to -\infty} V(x) = 0$ and $\lim_{x \to +\infty} V(x) = +\infty$, so that the region $x \to \infty$ is not accessible at finite energy. It is easy to find the right boundary conditions for $\psi_{1,2}$ for this case too. In the case of ψ_2 the condition is the same as before: outgoing plane wave. So we have again $\psi_2 \equiv \psi_-$. For ψ_1 the two possible behaviours at $x \to +\infty$ by solving the Schroedinger equation are exponentially growing or exponentially decreasing. We obviously must choose the second one to make physical sense. Then whe have that ψ_1 is just the stationary solution ψ_{stat} of the Schroedinger equation with energy E: it belongs to the physical Hilbert space. Notice on the other hand, that ψ_-, an outgoing wave at $x \to -\infty$, will always be, by current conservation, a combination of growing and decreasing solution at $x \to \infty$. Obviously ψ_- does not belong to the physical Hilbert space. But this does not concern the asymptotic behaviour of K because of the θ step functions in eq. (3.63). In this case the propagator is then

$$K(E; x, y) = \frac{2mi}{\hbar W} \left(\theta(x-y)\psi_{stat}(x)\psi_-(y) + \theta(y-x)\psi_-(x)\psi_{stat}(y) \right) \quad (3.74)$$

The last case to consider is the one where motion is fully limited: $\lim_{|x| \to +\infty} V(x) = +\infty$. In this case both ψ_1 and ψ_2 must correspond, at any real value of E, to the exponentially dcreasing solutions at respectively $x \to +\infty$ and $x \to -\infty$.

To illustrate our results let us consider the simplest possibe case of a free particle: $V(x) \equiv 0$. We have:

$$\begin{cases} \psi_1(x) = e^{ikx} \\ \psi_2(x) = e^{-ikx} \end{cases} \quad (3.75)$$

where $k = \sqrt{2mE}$.

We then get the fixed energy retarded propagator for the free particle:

$$\begin{aligned} K(E; x, y) &= \frac{m}{\hbar k} \left(\theta(x-y)e^{ik(x-y)} + \theta(y-x)e^{ik(y-x)} \right) \\ &= \frac{m}{\hbar k} e^{ik|x-y|} \end{aligned} \quad (3.76)$$

Which is precisely the expression derived in Homework 6, by inserting a complete set of fixed momentum states in eq. (3.59) and performing the momentum integral using Cauchy theorem. Notice that we recover a result similar to the correlator $G_\beta(\tau_1, \tau_2)$ in the limit $\beta \to \infty$.

Now, when we switch on the potential, we will have to find the two following solutions to the Schrödinger equation:

$$\begin{cases} \psi_1 \equiv \psi_+(x) \to A_+ e^{ikx} & x \to +\infty \\ \psi_2 \equiv \psi_-(x) \to A_- e^{-ikx} & x \to -\infty \end{cases} \quad (3.77)$$

We will then define the retarded propagator by:

$$K(E; x, y) = \frac{2mi}{\hbar W} \left(\theta(x-y)\psi_+(x)\psi_-(y) + \theta(y-x)\psi_+(y)\psi_-(x) \right) \quad (3.78)$$

Example: Barrier penetration

With the potential $V(x)$ switched on, assuming that it has a barrier located somewhere along the x axis, we need $\psi_{1,2}$ to correspond to the solutions to the Schrödinger equation with the following asymptotic behaviour:

$$\psi_1 \equiv \psi_+(x) \rightarrow \begin{cases} e^{ikx} + B_+ e^{-ikx} & x \rightarrow -\infty \\ A_+ e^{ikx} & x \rightarrow +\infty \end{cases}$$

$$\psi_2 \equiv \psi_-(x) \rightarrow \begin{cases} A_- e^{-ikx} & x \rightarrow -\infty \\ e^{-ikx} + B_- e^{ikx} & x \rightarrow +\infty \end{cases}$$

where A_+ is the transmission coefficient giving the transmission probability $p = |A_+|^2$. Conservation of the probablity current moreover implies $|A_+|^2 + |B_+|^2 = 1$. The physical interpretation of the solution ψ_+ is that it describes an incoming wave $\psi_{in} = e^{+ikx}$ travelling from $-\infty$ which is scattered at the barrier into an outgoing wave ψ_{out} with $\psi_{out} = B_+ e^{-ikx}$ for $x \rightarrow -\infty$ and and $\psi_{out} = A_+ e^{+ikx}$ for $x \rightarrow +\infty$. Similarly for motion in the opposite direction described by ψ_-. We can compute the Wronskian at $x \rightarrow -\infty$: $W = 2A_- ik$. This gives:

$$K(E; x, y) = \frac{m}{\hbar k} \frac{1}{A_-} \left[\theta(x - y) \psi_+(x) \psi_-(y) + \theta(y - x) \psi_-(x) \psi_+(y) \right] \quad (3.79)$$

Now, in the limit $x \rightarrow \infty$, $y \rightarrow -\infty$, we find:

$$K(E; x \rightarrow \infty, y \rightarrow -\infty) = \frac{m}{\hbar k} A_+ e^{ik(x-y)} = \frac{A_+}{v} e^{ik(x-y)} \quad (3.80)$$

where $v = k/m$ is the velocity.

Thus, K directly gives the transmission coefficient: the propagator (as it should!) directly gives the amplitude for propagation through the barrier. Using the above definitions, $K(E; x, y)$ is written, in the limit $x \rightarrow \infty$, $y \rightarrow -\infty$, in an intuitive and concise way: $K(E, x, y) \rightarrow \frac{1}{v} \psi_{out}(x) \psi_{in}^*(y)$.

Similarly, one can consider reflexion by a barrier by letting $y \rightarrow -\infty$, $x \rightarrow -\infty$, and $x > y$. Far away, where $V(x) \rightarrow 0$, we have:

$$K(E; x, y) \sim \frac{1}{v} (\underbrace{\psi_{in}(x)}_{\text{direct}} + \underbrace{\psi_{out}(x)}_{\text{reflected}}) \psi_{in}^*(y)$$

$$= \frac{1}{v} \left(e^{ik(x-y)} + B_+ e^{-ikx - iky} \right) \quad (3.81)$$

We see in the two contributions in the above equation the relics of the two possible classical paths: a direct path from y to x, and a path from y to x where the particle is reflected by the barrier, as is illustrated in figure 3.1. This will become more transparent in the semiclassical path integral approach.

3.2.2 Semiclassical computation of $K(E)$

Let us now turn to the computation of $K(E; x, y)$ in the semiclassical approximation. This is expected to be a good approximation when we can neglect
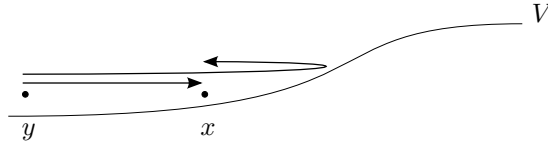
Figure 3.1: The two possible classical paths from y to x. The first one goes directly from y to x, whereas the second one is first reflected by the potential barrier before going to x.

derivatives higher than cubic in $V(x)$. Using the semiclassical result in eq. (3.44) we must perform a Fourier transform

$$K_{sc}(E; x_f, x_i) = \int_0^\infty \sqrt{-\frac{1}{2\pi i\hbar}\frac{\partial^2 S_c}{\partial x_i \partial x_f}}\; e^{i\frac{S_c}{\hbar} + \frac{iEt}{\hbar}}\, dt \qquad (3.82)$$

where the classical action S_c in a function of the initial and final positions x_i and x_f, and the travel time t.

For $\hbar \to 0$, or equivalently for E large enough, we expect a saddle point computation of the integral over t to be a reliable approximation. So we proceed with such a an evaluation. Notice that in doing so we are introducing an additional approximation in computing $K(E; x_f, x_i)$ with respect to the gaussian computation of $K(x_f, t; x_i, 0)$. In Problem 1 of Homework 7 the condition for the validity of these approximations is worked out.

Let us briefly recall how the saddle point approximation works.[4] We have to compute the following integral:

$$K = \int_0^\infty \sqrt{f(t)}\; e^{i\frac{g(t)}{\hbar}}\, dt \qquad (3.83)$$

In the limit where $\hbar \to 0$, this integral will be dominated by the region of the stationary point t_* where $g'(t) = 0$. In this region, we can substitute $f(t) \approx f(t_*)$ and $g(t) \approx g(t_*) + \frac{1}{2}g''(t_*)(t - t_*)^2$. We will get the following integral:

$$K = \sqrt{f(t_*)}e^{i\frac{g(t_*)}{\hbar}} \int_0^\infty e^{i\frac{1}{2}\frac{g''(t_*)}{\hbar}(t-t_*)^2}\, dt \qquad (3.84)$$

We will then be able to change the integration variable by $\delta t \equiv t - t_*$, and extend the lower bound of the integral from $-t_*$ to $-\infty$, thus getting an easily integrable Gaussian Integral.

Let us therefore look for the stationary point for the integral 3.82:

$$\left.\frac{\partial S_c}{\partial t}\right|_{t=t_*} + E = 0 \quad \Rightarrow \qquad (3.85)$$

$$-E_c(t_*) + E = 0 \quad \Rightarrow \quad t_* = t(E) \qquad (3.86)$$

where $E_c(t)$ is the energy of the classical trajectory for the motion from x_i to x_f in a time t, and t_* is the stationary point. Note that the the stationary point

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[4]**Notice** that we have already been using this concept throughout the course (in particular in sections 1.3.2 and 3.1). So the explanation given here should truly have been at the beginning! Better late than never.

approximation has selected a classical trajectory with energy $E_c = E$, showing that we are on the right track to derive a semiclassical approximation to the propagator.

We have that the exponent at the stationary point t_* is given by:

$$S_c + E_c t_* = \int_0^{t_*} \left(\mathcal{L} + E \right) dt = \int_0^{t_*} m\dot{x}_c^2 dt = \int_{x_i}^{x_f} p(x) dx \qquad (3.87)$$

where we used $S_c = \int (m\dot{x} dx - E dt)$ and where $p(x) = \sqrt{2m(E - V(x))}$ is the momentum of the classical trajectory with energy E.

Let us now find the second order expansion of S_c around t_* differentiating the identity $\frac{\partial S_c}{\partial t} = -E_c(t)$

$$\left. \frac{\partial^2 S_c}{\partial t^2} \right|_{t=t_*} = -\frac{\partial E_c}{\partial t} \qquad (3.88)$$

To explicitly write the result we need to use some simple mechanical identities. By using $\dot{x}_c = v(x) \equiv \sqrt{2(E_c - V(x))/m}$, we have

$$t = \int_{x_i}^{x_f} \frac{dx}{\dot{x}_c} = \int_{x_i}^{x_f} \sqrt{\frac{m}{2(E_c - V(x))}} dx$$

$$\Rightarrow 1 = -\frac{\partial E_c}{\partial t} \int_{x_i}^{x_f} \frac{1}{m} \left(\frac{m}{2(E - V(x))} \right)^{\frac{3}{2}} dx \qquad (3.89)$$

$$\Rightarrow -\frac{\partial E}{\partial t} = \frac{1}{\frac{1}{m} \int_{x_i}^{x_f} \frac{dx}{v^3}} = -v_i v_f \frac{\partial^2 S_c}{\partial x_i \partial x_f} \qquad (3.90)$$

where in the second step we differentiated with respect to t, and then set $t = t^*$, $E_c = E$ and where, again, $v_f = v(x_f)$ and $v_i = v(x_i)$.

The stationary phase integral is therefore:

$$\int d\delta t \exp \left(\frac{i}{2\hbar} \left(\frac{\partial^2 S_c}{\partial t^2} \right) (\delta t)^2 \right) = \sqrt{\frac{2\pi i \hbar}{\frac{\partial^2 S_c}{\partial t^2}}} = \sqrt{2\pi i \hbar \frac{1}{m} \int \frac{dx}{v^3}} \qquad (3.91)$$

Putting this into eq. (3.82), the final result is:

$$K(E; x_f, x_i) = \sqrt{\frac{1}{v(x_f)v(x_i)}} \exp \left(i \int_{x_i}^{x_f} \frac{p(x)}{\hbar} dx \right) \sim \psi_{WKB}(x_f)\psi_{WKB}^*(x_i) \qquad (3.92)$$

where we used the result eq. (3.73) to deduce the form of the fixed energy wave functions corresponding to our approximation

$$\psi_{WKB}(x) \sim \sqrt{\frac{1}{v(x)}} \exp \left(i \int_{x_0}^{x} \frac{p(x')}{\hbar} dx' \right) . \qquad (3.93)$$

This is the wave function which is derived in quantum mechanics by applying the Wentzel-Kramers-Brillouin (WKB) approximation. Problem 1 of Homework 7 is devoted to the standard derivation of the WKB approximation in the Schroedinger approach. That standard method also allows a direct study of the

domain of validity of the WKB approximation. The result is that one necessary requirement for WKB to be valid is

$$\frac{\hbar}{p^2(x)}\frac{dp}{dx} \equiv \frac{d\lambda(x)}{dx} \ll 1 \qquad (3.94)$$

corresponding to a physical situation where the De Broglie wavelength λ varies by a relatively small amount over a distance of order λ. Of course, keeping the classical parameters of the problem fixed, this requirement would be eventually satisfied by formally taking $\hbar \to 0$. This limit, where the wavelength goes to zero, is the quantum mechanics analogue of geometric optics limit for the propagation of electromagnetic waves. In that limit the propagation of light can be described by the propagation of particles along rays: the wavelength being small diffraction phenomena are negligible.

The above equation can also be written as a constraint on the force $F = -V'(x)$ acting on the particle

$$\frac{\hbar}{p^2(x)}\Big|\frac{dp}{dx}\Big| = \hbar\Big|\frac{mF}{p^3}\Big| \ll 1 \,. \qquad (3.95)$$

We thus see that at the points where the classical momentum is very small the WKB approximation breaks down. In particular this is so at the turning points of the classical motion where $E = V$ and $p = 0$. Now, in all interesting applications the wave function at the turning points is not directly needed, which is reassuring. However in practically all interesting applications, in order to compute the propagator or the wave function at points where the WKB approximation applies one still has to deal with matching conditions close to the turning points where the approximation breaks down. In the path integral formulation the issue arises in that one has to consider in the semiclassical computation of the propagator trajectories that go through turning points. The standard method to overcome the breakdown of the WKB approximation at the turning points is to deform the trajectory into the complex plane for the coordinate x (and for time t as well) in such a way as to avoid the point where $v(x) = 0$.

3.2.3   Two applications: reflection and tunneling through a barrier

In this section we shall consider two basic applications of the WKB propagator formalism. We shall not worry about the subtleties of reflection points, and compute whatever we can compute. Sections 3.2.4 and 3.2.5 will delve with more details into those issues.

Let us first examine the process of reflection by a potential barrier. This will be studied in detail in the exercises. Let us assume for that that we have a potential $V(x)$ that vanishes as $x \to -\infty$, and that has a barrier somewhere along the x axis. When we put $x_i, x_f \to -\infty$, $x_f > x_i$, the classical action from x_i to x_f accepts two solutions: one going directly from x_i to x_f, and one reflected first by the barrier at a and then going to x_f, as shown in figure 3.2.

Then, the Green's function will be decomposed into the contributions of the two classical paths: $K(E) = K_1 + K_2$. The contribution of the reflected path,
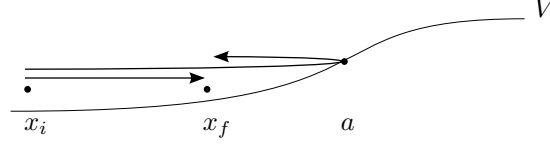
Figure 3.2: The two possible classical paths from x_i to x_f. The first one goes directly from x_i to x_f, whereas the second one is going first from x_i to a, and then is reflected from a to x_f.

K_2, is interesting because it contains information about the phase shift induced by the reflexion. K_1 is the same as without barrier.

It turns out that:

$$K_2(E; x_f, x_i) = \sqrt{\frac{1}{v(x_i)v(x_f)}} e^{-i\frac{\pi}{2}} \exp\left(\frac{i}{\hbar} \int_{x_i}^{x_f} p(x)dx_{(2)}\right) \qquad (3.96)$$

where $\int_{x_i}^{x_f} p(x)dx_{(2)} = \int_{x_i}^{a} |p(x)| \, dx + \int_{x_f}^{a} |p(x)| \, dx$ is the integral over the reflected path. $|p(x)|$ is defined as $\sqrt{2m(E - V(x))} > 0$.

The origin of the extra $-i$ factor is that $\det\left(-m\partial_t^2 - V''(x)\right) < 0$ over the reflected trajectory, or more precisely this operator has one negative eigenvalue.

Now, if we assume $x > y$, $x, y \to -\infty$, and remember eq. (3.74) we can write:

$$K(E; x, y) = K_1 + K_2 = \psi_{out}(y)\psi_{stat}(x)$$

$$= \sqrt{\frac{1}{v(x)v(y)}} \left(e^{\frac{i}{\hbar}\int_y^x |p(z)|dz} + e^{-i\frac{\pi}{2}}e^{\frac{i}{\hbar}\left(\int_y^a |p(z)|dz + \int_x^a |p(z)|dz\right)}\right)$$

$$= \sqrt{\frac{1}{v(x)v(y)}} e^{\frac{i}{\hbar}\int_y^a |p(z)|dz - i\frac{\pi}{4}} \left(e^{-\frac{i}{\hbar}\int_x^a |p(z)|dz + i\frac{\pi}{4}} + e^{\frac{i}{\hbar}\int_x^a |p(z)|dz - i\frac{\pi}{4}}\right)$$

$$= \sqrt{\frac{1}{v(y)}} e^{\frac{i}{\hbar}\int_y^a |p(z)|dz - i\frac{\pi}{4}} \cdot \sqrt{\frac{1}{v(x)}} \cos\left(\frac{1}{\hbar}\int_x^a |p(z)| \, dz - \frac{\pi}{4}\right) \quad (3.97)$$

Thus, we have found the physical eigenstate ψ_{stat} of the Schrödinger problem:

$$\psi_{out}(y) = \sqrt{\frac{1}{v(y)}} e^{\frac{i}{\hbar}\int_y^a |p(z)|dz - i\frac{\pi}{4}}$$

$$\psi_{stat}(x) = \sqrt{\frac{1}{v(x)}} \cos\left(\frac{1}{\hbar}\int_x^a |p(z)| \, dz - \frac{\pi}{4}\right) \qquad (3.98)$$

Imagine now, that the motion is bounded also to the "far" left at $b \ll a$. Applying the same argument, to a wave that is reflected at b we have the following result for ψ_{stat}

$$\psi_{stat(b)}(x) = \frac{1}{\sqrt{v(x)}} \cos\left(\frac{1}{\hbar}\int_b^x |p(z)| \, dz - \frac{\pi}{4}\right) \qquad (3.99)$$

Now, the two stationary solutions must coincide up to the sign, as they solve the same problem (energy bound eigenstate in one-dimensional Quantum

Mechanics). We have:

$$\psi_a(x) = \cos\left(\frac{1}{\hbar}\int_x^a |p(z)|\,dz - \frac{\pi}{4}\right) = \cos\left(\phi_a(x)\right)$$

$$\psi_b(x) = \cos\left(\frac{1}{\hbar}\int_b^x |p(z)|\,dz - \frac{\pi}{4}\right) = \cos\left(\phi_b(x)\right) \qquad (3.100)$$

Taking the derivatives, we find:

$$\partial_x \phi_a = -\partial_x \phi_b \quad \Rightarrow \quad \phi_a(x) + \phi_b(x) = \theta \qquad (3.101)$$

where θ is independent of x.

We then get:

$$\begin{aligned}
\psi_a(x) &= \cos\left(\phi_a(x)\right) \\
\psi_b(x) &= \cos\left(\theta - \phi_a(x)\right) = \cos\theta\cos\phi_a - \sin\theta\sin\phi_a \\
&\Rightarrow \theta = m\pi, \quad m \in \mathbb{Z} \\
&\Rightarrow \psi_a(x) = \pm\psi_b(x)
\end{aligned} \qquad (3.102)$$

This condition gives a constraint for the integral over the closed contour:

$$\oint p(z)dz = \frac{2}{\hbar}\int_b^a |p(z)|\,dz =$$
$$\frac{2}{\hbar}\int_b^x |p(z)|\,dz + \frac{2}{\hbar}\int_x^a |p(z)|\,dz = 2\pi\left(m + \frac{1}{2}\right) \quad (3.103)$$

This is the famous Bohr-Sommerfeld semi-classical quantization condition.

Barrier penetration: semiclassical transmission coefficient

Imagine now that the potential $V(x)$ has a barrier so that a classical particle with an energy E cannot go from $-\infty$ to $+\infty$ (see figure 3.3).
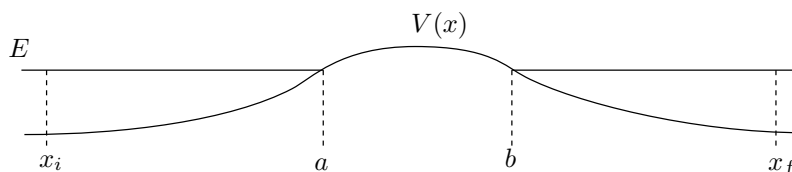

Figure 3.3: There is no classical trajectory going from x_i to x_f with an energy E. The potential barrier is too high to let a particle go past it. Quantum physics in the semi classical limit predict a non-vanishing probability for such a particle to tunnel through the barrier from x_i to x_f.

However, we can define a semiclassical contribution to this process, which can be seen in the WKB approximation. The equivalence between WKB and Gaussian approximation requires therefore to find the corresponding contribution in the path integral approach. Thus, we have to look for the stationary

point of the combined $\int \mathscr{D}[x]dt$ integral:

$$K(E; x_f, x_i) = \int_0^\infty \int \mathscr{D}[x] e^{\frac{i}{\hbar}(S_c + Et)} dt \qquad (3.104)$$

The result is that we can find a stationary point provided t is complex! Indeed, from the classical equation of motion, we find that:

$$\frac{dx}{dt} = \sqrt{\frac{2(E - V(x))}{m}} \qquad (3.105)$$

Considering extending this equation at $a < x < b$, we have:

$$\frac{dx}{dt} = +i\sqrt{\frac{2\,|E - V(x)|}{m}} \qquad (3.106)$$

where we chose the plus sign in order to ensure that the Green's function remain analytic.

Integrating over the full trajectory, we get:

$$t = \int dt = \int_{x_i}^{x_f} \underbrace{\sqrt{\frac{m}{2(E - V(x))}}}_{v(x)} dx$$

$$= \underbrace{\int_{x_i}^a \frac{dx}{v(x)}}_{\text{real}} - i\underbrace{\int_a^b \frac{dx}{|v(x)|}}_{\text{imaginary}} + \underbrace{\int_b^{x_f} \frac{dx}{v(x)}}_{\text{real}} \qquad (3.107)$$

The evolution of time in the complex plane along the trajectory is depicted in figure 3.4.
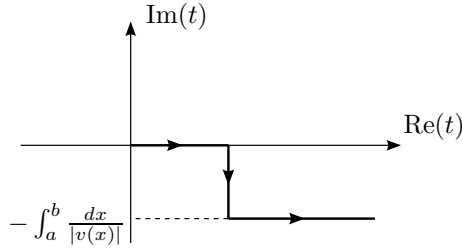

Figure 3.4: The evolution of the time along the trajectory in the complex plane. It acquires a negative imarinary part as the particle travels through the potential barrier.

Now, regardless of the course of the complex value of t, we still have:

$$\frac{i}{\hbar}(S_c(t) + Et)\bigg|_{\text{stat}} = \frac{i}{\hbar}\int_{x_i}^{x_f} \sqrt{2m(E - V(x))}dx \qquad (3.108)$$

The Jacobian factor from the gaussian integration around the extremum of

t still compensates the determinant:

$$K(E; x_f, x_i) = \sqrt{\frac{1}{v(x_f)v(x_i)}} \exp\left(\frac{i}{\hbar} \int_{x_i}^{x_f} \sqrt{2m(E - V(x))} dx\right)$$

$$= \underbrace{\sqrt{\frac{1}{v(x_i)}} e^{\frac{i}{\hbar} \int_{x_i}^{a} |p(x)| dx}}_{\psi_{in}^*} \underbrace{\sqrt{\frac{1}{v(x_f)}} e^{\frac{i}{\hbar} \int_{b}^{x_f} |p(x)| dx} \overbrace{e^{-\frac{1}{\hbar} \int_{a}^{b} |p(x)| dx}}^{A_+}}_{\psi_{out}}$$

$$(3.109)$$

where the transmission coefficient is given by A_+.

We can then derive the probability P of tunneling:

$$P = |A_+|^2 = e^{-\frac{2}{\hbar} \int_a^b |p(x)| dx} = e^{-\frac{2}{\hbar} \int_a^b \sqrt{2m(V(x) - E)} dx} \qquad (3.110)$$

3.2.4   On the phase of the prefactor of $K(x_f, t_f; x_i, t_i)$

We have so far been rather cavalier concerning the phase of our Gaussian integrals. However, as our previous discussion makes clear, when multiple trajectories contribute to the amplitude it is essential to be in control of their relative phases. In this subsection, we will give the basic idea for the case of $K(x_f, t_f; x_i, t_i)$. The next subsection is devoted to the phase of $K(E; x_f, x_i)$, which is very relevant to the discussion several applications like the computation of energy levels in the WKB approximation (see Homework 7).

1) Getting the basic idea

In order to get an idea, let us go back to the determinant prefactor for the harmonic oscillator which was computed in eq. (1.98). In that derivation we did not pay any real attention to the phase factors that arose when some eigenvalues became negative. Eq. (1.89) tells us that the number n_- of negative eigenvalues equals the integer part of $\omega T/\pi$ ($T \equiv t_f - t_i$). Thus for $0 < T < \pi/\omega$ we have $n_- = 0$ so that the phase of the prefactor is the same as for the free particle case. The specific phase of eq. (1.98) is only correct for this range of T. By eq. (1.58), for $n_- \neq 0$ the phase of the harmonic oscillator prefactor relative to that of the free particle is $\exp(-in_- \frac{\pi}{2})$. Therefore the correct result for the propagator prefactor is given by

$$J_\omega(T) = e^{-in_- \frac{\pi}{2}} \sqrt{\frac{m\omega}{2\pi i\hbar |\sin(\omega T)|}} \qquad (3.111)$$

rather than by eq. (1.98). Thus when T increases by a half-period π/ω the propagator aquires an extra phase factor $= -i$. With an extra full period $2\pi/\omega$ the propagator just flips sign: $(-i)^2 = -1$. This result can also be stated as

1. For trajectories in which the velocity does not flip sign there is no extra phase factor

2. For trajectories where the velocity flips sign n times the phase is either $e^{in\pi/2}$ or $e^{i(n-1)\pi/2}$ (depending on how many multiples of the half period fit into T)

3. For a trajectory corresponding to exactly k periods of motion the phase factor is $(-1)^k$

This result is valid for any periodic motion not just for the harmonic oscillator. There is a well developed mathematical theory, called Morse theory, underlying the dependence of the number of negative eigenvalues n_- on the properties of the trajectory. n_- is referred to as the *Morse index*. We are not going to linger on this mathematical connection though. A simple paper with some more details is for instance ref. [9].

2) An explicit non trivial example [5]

$$V(x) = \theta(x)\frac{m\omega^2}{2}x^2$$

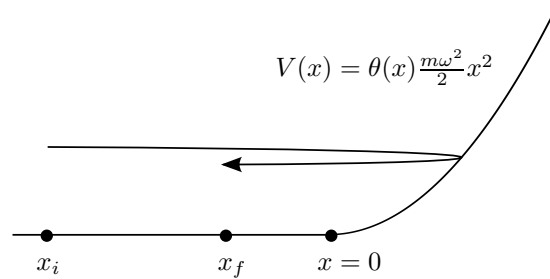$x_i \qquad x_f \qquad x = 0$

Figure 3.5: .

Let us see now a slightly less straightforward case by considering the motion in the potential $V(x) = \theta(x)\frac{1}{2}m\omega^2 x^2$ shown in fig.3.5. The novelty with respect to the harmonic oscillator is that the motion at $x < 0$ is not bounded, so that motion is not periodic. Let us compute the fluctuation determinant using eqs. (3.15, 3.16). We also want to do so by focusing on a 1-dimensional family of trajectories characterized by initial position $x(0) = x_i < 0$ and velocity $\dot{x}(0) \equiv v > 0$ at $t = 0$. The classical motion is characterized by 3 time, t, intervals

1. For $0 \le t \le -\frac{x_i}{v} \equiv t_1$ we have $x(t) = x_i + vt \le 0$: the particle moves in the $V(x) = 0$ region with positive velocity.

2. For $t_1 < t < t_1 + \frac{\pi}{\omega}$ we have $x(t) = \frac{v}{\omega}\sin[\omega(t - t_1)]$: the particle moves in the harmonic potential at $x > 0$.

3. For $t \ge t_1 + \frac{\pi}{\omega}$ the trajectory is again "free", $x(t) = -v(t - t_1 + \frac{\pi}{\omega}) < 0$ but the velocity is now negative.

We want to compute the determinant function $\psi_0(t_f)$ as t_f is varied in the above 3 intervals. The operator controlling the quadratic fluctuation is

$$-m\frac{d^2}{dt^2} - V''(x(t)) = -m\frac{d^2}{dt^2} - m\omega^2\theta(t - t_1)\theta(t_1 + \frac{\pi}{\omega} - t) \qquad (3.112)$$

where the product of step functions accounts for the fact that $V \neq 0$ only for $t_1 < t < t_1 + \frac{\pi}{\omega}$. The initial value problem in eqs. (3.15, 3.16) for the differential

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[5]This problem was proposed in one of the exercise sessions.

operator 3.112 is solved by patching the solution in the 3 time regions listed above. In other words, first the solution in region 1 is found. Second, the solution in region 2 is found with initial conditions at $t = t_1$ dictated by continuity of ψ_0 and $\dot{\psi}_0$. Third this procedure is repeated to get the solution in region 3. One finds respectively in region 1, 2 and 3

1. For $0 \leq t \leq -\frac{x_i}{v} \equiv t_1$ the solution is $\psi_0(t) = t$

2. For $t_1 < t < t_1 + \frac{\pi}{\omega}$ one has: $\psi_0(t) = \sqrt{\frac{1}{\omega^2} + t_1^2} \sin[\omega(t - t_1) + \varphi]$ where $0 \leq \varphi \leq \pi/2$ is defined by $\tan \varphi = \omega t_1$. Notice that $\psi_0(t_1 + \pi/\omega) = -\psi_0(t_1) = -t_1 < 0$.

3. For $t \geq t_1 + \frac{\pi}{\omega}$ one has finally $\psi_0(t) = -t + \frac{\pi}{\omega} < 0$

Let us now increase t_f starting from $t_f < t_1$. By the above result we have that the determinant $\psi_0(t_f)$ is positive and grows with t_f in region 1. Indeed not only is the determinant positive in region 1, but all eigenvalues are positive. This is because for $t_f < t_1$ eq. (3.112) reduces to the free particle quadratic fluctuation which is a positive definite differential operator, as we already know very well. At some $t_f = t_*$ in region 2, $t_1 < t_* < t_1 + \pi/\omega$, the determinant crosses zero once and becomes negative. In region 3, $\psi_0(t_f)$ decreases and thus stays negative without ever reaching zero again. The picture of what happens is then obvious:

- For $t_f < t_*$ the eigenvalues are all positive $0 < \lambda_1 < \lambda_2 < \lambda_3 < \ldots$

- At $t_f = t_*$ the smallest eigenvalue λ_1 vanishes, and for any $t_f > t_*$ the spectrum satisfies $\lambda_1 < 0 < \lambda_2 < \lambda_3 < \ldots$: there is one and only one negative eigenvalue.

For $t_f > t_*$ the gaussian integral prefactor is then (compare to eq. (3.28))

$$I[x_c] = e^{-i\frac{\pi}{2}} \sqrt{\frac{m}{2\pi i \hbar |\psi_0(t_f)|}} \tag{3.113}$$

Another comment concerns the point at which the determinant flips sign. Notice that this happens at t_* strictly larger than the time $t_r = t_1 + \frac{\pi}{2\omega}$ at which reflection by the potential barrier happens. That is to say: $\psi_0 > 0$ before reflection. This is a general result that can be easily seen by using the integral formula in eq. (3.32). From that equation is it obvious that $\psi_0 > 0$ for trajectories in which the velocity does not flip sign. Let us show that a stronger result holds, namely $\lim_{t_f \to t_r} \psi_0(t_f) > 0$ when t_f approaches t_r from below. For $t \to t_r$ the velocity goes to zero linearly: $v(t) \simeq a(-t + t_r)$, with a a positive coefficient (so that the acceleration is $\dot{v} = -a < 0$). Then the integral in eq. (3.32) diverges but its prefator $v_f v_i$ goes to zero so that the result is finite

$$\lim_{t_f \to t_r} \left\{ v(t_f)v(t_i) \int_{t_i}^{t_f} \frac{1}{v_c^2(t)} dt \right\} = \tag{3.114}$$

$$\lim_{t_f \to t_r} v(t_i)a(-t_f + t_r) \left[\frac{1}{a^2} \frac{1}{-t_f + t_r} + \text{finite} \right] = \frac{v(t_i)}{a} > 0 \tag{3.115}$$

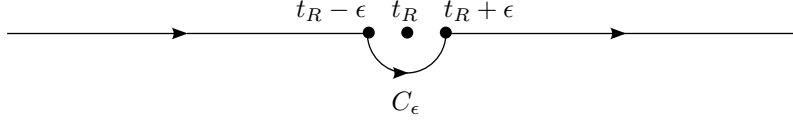and therefore the determinant can only flip sign after reflection.

Figure 3.6: .

3) The integral expression for ψ_0 and reflecting trajectories

One final remark concerns the way to make sense of eq. (3.32) and eq. (3.34) in the case of trajectories where v does change sign. These equations are ill defined in such cases: the factor $v_f v_i$ is non-zero, but the integral diverges at the points where $v \to 0$. This is because in deriving them we had to divide by v somewhere. Notice however that no singularity should exist in ψ_0 is association to the vanishing of the velocity. This is because ψ_0 is just given by the solution of an ordinary differential equation with finite coefficients. This suggest that be should be able to 'save' eq. (3.32) and eq. (3.34). The way to do so is very simple: we just need to slightly deform the trajectory into the complex (x, t) plane in such a way as to avoid the singularities. When working with the time integral eq. (3.32), by eq. (3.115) we see that the integrand has a double pole: we just need to go around it as shown in fig. 3.6. Notice also that it does not make any difference to go around the pole from below, as in the figure, or from above. This is because the singularity is a *double pole* and thus the integral over a full oriented circle around it gives zero by Cauchy's theorem. The integral on the oriented half circle contour C_ϵ is easily computed for $\epsilon \to 0$ by parametrizing $t - t_r = -\epsilon e^{i\theta}$, with $0 \le \theta \le \pi$ on C_ϵ, so that $dt = -i\epsilon e^{i\theta} d\theta$. We have

$$\lim_{\epsilon \to 0} \int_{C_\epsilon} \frac{dt}{v^2(t)} = \int_{C_\epsilon} \frac{dt}{a^2 (t - t_r)^2} = \tag{3.116}$$

$$\frac{1}{\epsilon a^2} \int_0^\pi -i e^{-i\theta} d\theta = \frac{1}{\epsilon a^2} \left[-1 - 1 \right] . \tag{3.117}$$

This result precisely cancels the diverge of the integrals at $t < t_r - \epsilon$ and $t > t_r + \epsilon$ so that we have in the end

$$\psi_0 = v_i v_f \lim_{\epsilon \to 0} \left\{ \left[-\frac{1}{\epsilon a^2} + \int_{t_i}^{t_r - \epsilon} \frac{dt}{v^2(t)} \right] + \left[-\frac{1}{\epsilon a^2} + \int_{t_r + \epsilon}^{t_f} \frac{dt}{v^2(t)} \right] \right\} \tag{3.118}$$

We can also change variable $t \to x$. The reflection point x_r is defined by $v(x_r) = \sqrt{2(E - V(x_r))/m} = 0$, where E is the energy of the trajectory in consideration. The equation of motion gives $V'(x_r)/m = a$. Then we have that $t_r \pm \epsilon$ both correspond to $x_r - \frac{a}{2}\epsilon^2$ so that the above equation becomes

$$\psi_0 = v_i v_f \left\{ \left[-\frac{1}{\epsilon a^2} + \int_{x_i}^{x_r - \frac{a}{2}\epsilon^2} \frac{dx}{|v^3(x)|} \right] + \left[-\frac{1}{\epsilon a^2} + \int_{x_f}^{x_r - \frac{a}{2}\epsilon^2} \frac{dx}{|v^3(x)|} \right] \right\} \tag{3.119}$$

Using this formula, we can study the conditions on $V(x)$ under which ψ_0 flips sign after reflection. Since for a reflecting trajectory $v_i v_f < 0$, we have that ψ_0 is negative if and only if the expression in curly bracket is positive. Now, if the potential at $x \to -\infty$, i.e. in the classically accessible region, is flat enough, then

it is obvious that, for x_i or x_f large enough and negative, the expression in curly brakets is dominated by the positive integral in the region away from the turning point. Thus we have $\psi_0 < 0$. However if $\lim_{x\to-\infty} V(x) = -\infty$ fast enough, then $\int dx/v^3$ is dominated by the region close to the turning point. In this case the expression in curly braket does not necessarily become positive for large enough x_i and x_f and ψ_0 may never flip sign. A simple and obvious example where this is so is given by the linear potential $V = cx$. This is obvious because in this case $V'' = 0$ and we have the free particle result $\psi_0(t_f) = t_f - t_i > 0$.

It is a good exercise to recover the result we found for ψ_0 in the potential in fig. 3.5 by using instead the integral representation of ψ_0. We shall not do that but just give some suggestions on how to try and do it. Using the space integral representation eq. (3.34), one notices that $v(x)$ has a cut in the complex x plane along the x region accessible to classical motion. Physically this corresponds to the velocity being double valued: $v(x) = \pm\sqrt{2(E - V(x))/m}$. Then ψ_0 is computed on a trajectory that goes around this cut...The willing student can now go ahead and make a simple remark (on Cauchy integrals) that allows for a direct computation.

3.2.5   On the phase of the prefactor of $K(E; x_f, x_i)$

Let us now focus on the phase of $K(E; x_f, x_i)$, which is really what matters in most applications. Again the delicate issue is how to deal with the turning points. Two basic remarks are in order here.

The first is that for x_i or x_f close to the turning points, the WKB approximation to $K(E; x_f, x_i)$ breaks down[6] because $p(x) \to 0$ (see eq. (3.95)). The saddle point approximation can however still be reliable if the trajectory can be deformed into the complex $\mathbb{C}^2$ plane for (t, x) in such a way that $p(x)$ never really crosses zero. In order for this procedure to makes sense two conditions must be satisfied (see the discussion in the chapter on the WKB approximation in Landau-Lifshitz [10])

- The potential $V(x)$ is analytic in a region around the turning point. This way, $v(x) = \sqrt{2(E - V(x))/m}$ is also analytic in this region apart from having a cut (due to the square root) in the physically accessible region on the real x axis.

- The region of analyticity for $V(x)$ overlaps with the region where the WKB approximation applies, that is with the region where $\hbar|mV'(x)/p(x)^3| \ll 1$.

When the above two conditions are satisfied, a suitable deformation of the trajectory can be chosen such that x goes around the turning points in such a way that: 1) Physical quantities, like the action integral, are unaffected by the deformation of the trajectory thanks to analyticity. 2) $p(x)$ is never too small

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[6]We stress that the situation is different with respect to the apparent singularity of $\psi_0(t_f)$ at the turning points which we encountered in the previous section. The gaussian approximation for $K(x_f, t_f; x_i, t_i)$ does not really break down in the presence of turning points, witness the fact that this approximation is exact for the harmonic oscillator. Instead the WKB computation of $K(E; x_f, x_i)$, as we already pointed out, requires an extra approximation, which genuinely breaks down at the turning points.

and the WKB is manifestly valid.[7]

We will explain with an example below how the deformation works. Notice, for the moment, that by deforming the time line into the complex plane (like we did for instance with barrier penetration), the trajectory $x(t)$ which is defined to solve

$$m\frac{d^2x}{dt^2} = -V'(x)\,, \tag{3.120}$$

is also, in general, deformed into the complex x plane.

The second remark concerns the form of the prefactor itself. By continuing the trajectory into the complex plane we can still make sense of the integral $\int dx/v^3$ even when the velocity flips sign somewhere. Then, as we already know, all is left in the prefactor is the velocity at the initial and final points

$$P(x_f, x_i) = \sqrt{\frac{-1}{2\pi i\hbar}\frac{\partial^2 S_c}{\partial x_f \partial x_i}} \cdot \sqrt{\frac{2\pi i\hbar}{\frac{\partial^2 S_c}{\partial t^2}}} = \sqrt{\frac{1}{v(x_f)v(x_i)}}\,. \tag{3.121}$$

Since $v(x_f)$ changes sign at the turning point, the above prefactor gains a $1/\sqrt{-1}$ factor precisely at reflection. The only question is that $1/\sqrt{-1}$ being double valued, we cannot yet tell, simply by staring at eq. (3.121), if the phase is $+i$ or $-i$. Also, just by staring at the above equation, it is not obvious how to proceed for trajectories with multiple reflections. It turns out that the right answer is:

- At each reflection the prefactor gains a phase factor $(-i) = e^{-i\pi/2}$.

This result can be directly and easily checked for the example we discussed in section 3.2.4, using the computations we have already made. There are two contributions to the phase. One is the phase of the VanVleck-Pauli-Morette prefactor in eq. (3.113). We computed this phase factor in section 3.2.4 and found that it is $e^{-i\pi/2}$ for x_f and x_i negative. The second comes from the phase of the gaussian integral over t and is determined by the sign of $\partial^2 S/\partial t^2$. It is easy to see that $\partial^2 S/\partial t^2 > 0$. Indeed by eqs. (3.88) and (3.90) we have that $\partial^2 S/\partial t^2$ is just the inverse of the expression in curly brackets in eq. (3.119). In the case at hand that expression is clearly positive since, $v_i v_f < 0$ and since $\psi_0(t_f) < 0$ by our direct solution of the differential equation. Since $\partial^2 S/\partial t^2$ is positive, like for a non-reflecting trajectory, the phase of the t integral is trivial and the only non trivial contribution is that from the determinant, which equals $e^{-i\pi/2}$. This is in agreement with the general result we stated above

There is one quick way to deduce in general that for $v_i v_f < 0$ the phase in eq. (3.121) must be $e^{-i\pi/2}$. Without loss of generality and to simplify the discussion let us consider a particle of mass $m = 1$, let us shift the definition of the energy such that $E = 0$ for our trajectory, let us shift x so that the turning point is $x_r = 0$ and let us choose $V(x) \simeq x$ in the vicinity of $x = 0$. The equation of motion close to $x = 0$ is just

$$\ddot{x} = -1 \tag{3.122}$$

where again, without loss of gererality, we can focus on the solution $x = -\frac{1}{2}t^2$ with $v \equiv \dot{x} = -t$. For real t the velocity flips sign at $t = 0$. If we deform t into

---

[7]Notice that the time contour shown in fig.3.6 are an example of how to go around turning points. To be manifestly in the WKB approximation ϵ should be large enough. However because of analyticity the result of all integrals is independent of ϵ anyway!

$$t = 0$$

$$-i\epsilon$$
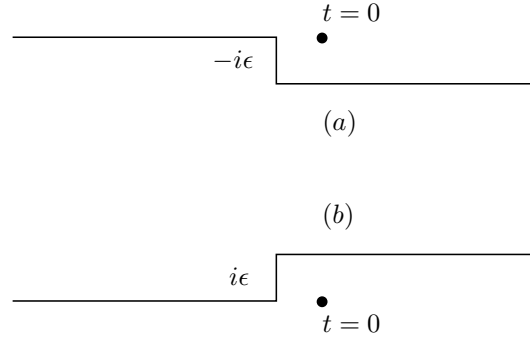
$$(a)$$

$$(b)$$

$$i\epsilon$$

$$t = 0$$

Figure 3.7: .

the complex plane we have two options to go around the point $t = 0$ where the velocity vanishes. Either we go below like in fig. 3.7a or above like in fig. 3.7b. These two options lead to different (and conjugate) phase shifts for $1/\sqrt{v(t_f)}$. Which of the two deformations should we choose? It turns out deformation (a) is acceptable while (b) is not. To understand why, we should go back and think what it means to deform t into complex values in our original definition of the path integral. It means that, rather than doing our simple (and real) slicing $dt = (t_f - t_i)/N$, we are making some element dt of the sum $\int dt = t_f - t_i$ complex. As long as we write $U(t_f - t_i)$ as a product of matrices this is not a problem. A constraint arises however when we attempt to write this product of matrices in terms of a path integral as done in section 1.1.4. This is because if $\mathrm{Re}\,(-idt) > 0$ in the exponent $e^{(-iHdt/\hbar)}$, then the p integral in eq. (1.14) is not convergent: it is growing at $p \to \infty$ (the ϵ interval of that equation corresponds to our dt). This is just an infinitesimal way of saying that the euclidean path integral exists only for $\beta > 0$. Since our semiclassical approximation is based on a path integral representation of the evolution amplitude, we should only consider trajectories (real or complex) for which the path integral representation makes sense. That is to say only trajectories such that $\mathrm{Im}\,(dt) \leq 0$. This the case for trajectory (a) and not the case for trajectory (b). We are now just left with computing the phase shift in $1/\sqrt{v(t)} = 1/\sqrt{-t}$ along trajectory (a). When t goes from $-\infty$ to $+\infty - i\epsilon$ the argument in $\sqrt{-t}$ goes from $+\infty$ to $-\infty + i\epsilon$ by passing in the upper half plane, therefore the phase of $\sqrt{-\infty + i\epsilon}$ is $e^{i\pi/2}$. The resulting phase of the prefactor is then

$$\frac{1}{\sqrt{v(-\infty + i\epsilon)}} = e^{-i\pi/2}\frac{1}{\sqrt{|v(-\infty)|}} \tag{3.123}$$

More formally we can compute the phase shift $\Delta\varphi$ by integrating over the t contour

$$\Delta\varphi \equiv \mathrm{Im}\,\Delta\left[\ln(1/\sqrt{v})\right] = -\mathrm{Im}\int\frac{dv}{2v} = -\mathrm{Im}\int_{-\infty}^{+\infty - i\epsilon}\frac{dt}{2t} = -\frac{1}{2}\pi = -\frac{\pi}{2} \tag{3.124}$$

Chapter 4

Instantons

4.1 Introduction

In Quantum Mechanics, perturbation theory can miss important features of a physical system.

To illustrate this, let us give a quick look at a simple example: a one-dimensional particle in a potential $V(x) = \frac{m\omega^2 x^2}{2} + \lambda x^3$.

The point $x = 0$ is a classical minimum and it seems reasonable to study the dynamics around this point upon quantization. For λ "small" enough, we can apply perturbation theory and in principle compute the ground state energy to any desired order in λ. In doing so, however, we would not realize, or get any direct indication of one basic pathology of this ground state: its instability! Due to the possibility of tunneling through the barrier, the ground state will be able to decay down to the region where λx^3 is negative and dominates the harmonic term (see figure 4.1).
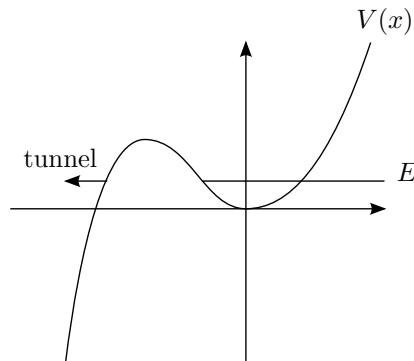

Figure 4.1: The stability of the ground state localized around the local minimum of the potential is broken by the possibility for the particle to tunnel through the barrier to the part of the potential unbounded from below.

The probability of tunneling will be proportional to: $P \sim \exp\left(-2 \int \frac{\sqrt{Vm}}{\hbar} dx\right) \sim \exp\left(-\frac{m^3 \omega^5}{\hbar \lambda^2}\right)$. It thus represents an effect which vanishes, as $\lambda \to 0$, faster that

any power of λ, implying that it cannot be seen at any finite order in perturbation theory. This is what theorists normally call a non-perturbative effect.

As a second example, let us look at the case of a particle in a double well potential: $V(x) = \lambda(x^2 - a^2)^2$ symmetric under reflection $x \to -x$ (see figure 4.2).

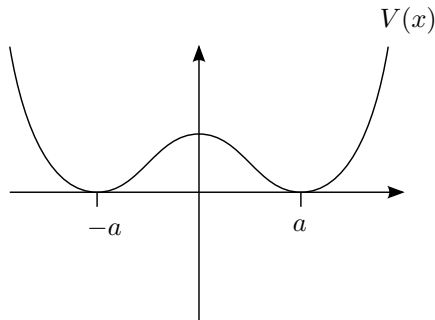Figure 4.2: The double well potential has two relexion symmetric vacua, thus leading to inexistant degenerate eigenstates in perturbation theory.

This potential has two classical ground states: $x = \pm a$, which are equivalent because of the reflection symmetry of the system. In perturbation theory, we can ignore this doubling and expand around one of these minima, say $x = a$. We introduce thus the new variable $y = x - a$. In this variable, $V(y)$ is a harmonic oscillator with extra cubic and quartic terms which we can treat as perturbations as long as λ is "small". We have:

$$V(y) = \lambda \left(y + 2a\right)^2 y^2 \quad = \quad 4\lambda a^2 y^2 + 4\lambda a y^3 + \lambda y^4 \tag{4.1}$$

$$\equiv \quad \frac{1}{2} m\omega^2 y^2 + \omega\sqrt{2m\lambda}\, y^3 + \lambda y^4 \tag{4.2}$$

where in the last equation we traded a for the harmonic oscillator frequency ω. For small λ, we can now compute the corrections to the lowest energy levels to arbitrary orders in λ without having any direct evidence that there is another minimum with its own localized levels!

The situation is here symmetric: a guy sitting at the other classical ground state would compute in perturbation theory exactly the same levels[1] , but corresponding to a different set of states where the wave function is localized near $x = -a$ instead of $x = a$. Thus, in perturbation theory, the energy levels, and in particular the ground state, are all doubly degenerate to all orders.

However, from the exact quantum mechanical solution of the problem, we know that for a unidimensional system, there is no degeneracy of the bound state energy eigenvalues. Moreover, we know that the ground state wave function has no nodes, and, in the case at hand, is therefore even under $x \to -x$:

$$\Psi_0(x) = \Psi_0(-x)$$

---

[1]Technically, this other guy expands the coordinate as $x = -a - y'$. Because of reflection symmetry the potential in y' satisfies $V(-a - y') = V(a + y')$: exactly the form in eq. (4.1). Hence the levels, in perturbation theory, are the same.

On the other hand, the first excited state has one node, and must therefore be odd under reflection:

$$\Psi_1(x) = -\Psi_1(-x)$$

However, because of the doubling of all the levels that we just deduced with our perturbative reasoning, the energy eigenvalues of these two lowest lying states mus be degenate to all orders in perturbation theory. That is $E_1 - E_0 = 0$ to all orders in perturbation theory. The goal of this chapter is to show that the leading contribution to $E_1 - E_0$ as $\lambda \to 0$ can be computed by semiclassical methods. More precisely, via semiclassical trajectories in imaginary time called instantons.

4.2 Instantons in the double well potential

What we want to study are the properties of the ground state(s) of the double well potential: $V(x) = \frac{\lambda}{4!}\left(x^2 - a^2\right)^2$. To do this, let us go back to the Euclidean path integral.

We will compute $\langle a| e^{-\frac{\beta H}{\hbar}} |a\rangle$ and $\langle -a| e^{-\frac{\beta H}{\hbar}} |a\rangle$ for $\beta \to \infty$. If the barrier is high and the the potential smooth, we can perform a semiclassical approximation in Euclidean time.

To compute those two transition amplitudes, we must sum over all possible stationary trajectories (i.e. with stationary action) in Euclidean time.

Remember that:

$$\langle x_f| e^{-\frac{\beta H}{\hbar}} |x_i\rangle = K_E(x_f, x_i; \beta) = \int_{x_i, -\frac{\beta}{2}}^{x_f, \frac{\beta}{2}} \mathscr{D}[x] e^{-\frac{S_E[x]}{\hbar}} \tag{4.3}$$

$$S_E[x] = \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau \left(\frac{m\dot{x}^2}{2} + \frac{\lambda}{4!}\left(x^2 - a^2\right)^2\right) \tag{4.4}$$

For each trajectory $\bar{x}$, we can compute its contribution to K_E in Gaussian approximation:

$$K_E = \tilde{\mathcal{N}} \left(\det\left(-m\frac{d^2}{d\tau^2} + V''(\bar{x})\right)\right)^{-\frac{1}{2}} e^{-\frac{S_E[\bar{x}]}{\hbar}}(1 + \mathcal{O}(\hbar)) \tag{4.5}$$

Notice that S_E is positive definite. Now,

$$K_E = \int \mathscr{D}[x] e^{-\frac{S_E[x]}{\hbar}} \tag{4.6}$$

is dominated by the local minima of $S_E[x]$ with given boundary conditions:

$$x_f = x\left(\frac{\beta}{2}\right)$$

$$x_i = x\left(-\frac{\beta}{2}\right) \tag{4.7}$$

Imposing now that $\frac{\delta S_E}{\delta x} = 0$ leads to the Euclidean equation of motion. Notice that the solutions to this equation describe motion in the euclidean time
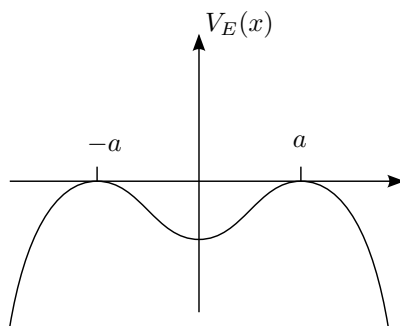
Figure 4.3: The Euclidean equation of motion corresponds to the real time equation of motion with a reversed potential $V_E(x) = -V(x)$.

parameter τ of a classical system with reversed potential $V_E(x) = -V(x)$ (see figure 4.3).

In the limit $\hbar \to 0$, we therefore expect K_E to be dominated by the local minima of S_E (if there exist more than one).

$$K_E \approx K_1 + K_2 + K_3 + \ldots \qquad (4.8)$$

Remark: we can make an analogy with the ordinary integrals. Suppose that we have a function $S(x)$, as depicted in figure 4.4.
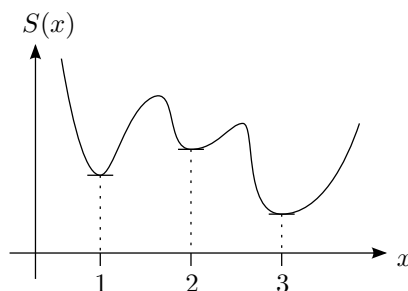

Figure 4.4: An ordinary function of one variable $S(x)$, accepting three local minima called 1, 2 and 3.

Then, in the limit $\hbar \to 0$, the integral

$$I = \int_{-\infty}^{\infty} e^{-\frac{S(x)}{\hbar}} dx \qquad (4.9)$$

can be approximated by

$$I \approx I_1 + I_2 + I_3 + \ldots$$

$$I_i = e^{-\frac{S(x_i)}{\hbar}} \sqrt{\frac{2\pi\hbar}{S''(x_i)}} \qquad (4.10)$$

The anharmonic terms around the local minima give corrections to each I_i of relative size $\hbar$.

To compute the transition amplitudes $\langle a| e^{-\frac{\beta H}{\hbar}} |a\rangle$, $\langle -a| e^{-\frac{\beta H}{\hbar}} |-a\rangle$, $\langle -a| e^{-\frac{\beta H}{\hbar}} |a\rangle$ and $\langle a| e^{-\frac{\beta H}{\hbar}} |-a\rangle$, we must study the classical trajectories in the upside down potential $V_E(x) = -V(x)$, depicted in figure 4.3.

This potential accepts two types of solutions:

Trivial solutions: $x(\tau) \equiv \pm a$ which will give the leading contribution to the first two amplitudes.

Less trivial solutions: the instanton, which starts at $x = -a$ at $\tau = -\infty$ and rolls towards $x = a$ at $\tau = \infty$, and the anti-instanton, which rolls from a to $-a$. These solutions are exact in the $\beta \to \infty$ limit.

The action on the instanton can be computed: as the initial velocity $\dot{x}(-\infty)$ is zero, then the Euclidean energy E_E is zero, and we can write:

$$\frac{m\dot{x}^2}{2} - V(x) = E_E = 0 \tag{4.11}$$

This allows us to write an expression for the Euclidean action:

$$\frac{m\dot{x}^2}{2} = V(x) \quad \Rightarrow \quad \dot{x} = \sqrt{\frac{2V(x)}{m}}$$

$$S_E = \int_{-\infty}^{\infty} m\dot{x}^2 d\tau = \int_{-a}^{a} m\sqrt{\frac{2V(x)}{m}} dx = \int_{-a}^{a} \sqrt{2mV(x)} dx \tag{4.12}$$

Thus, in the semiclassical limit, the transition amplitude will be proportional to:

$$\langle a| e^{-\frac{\beta H}{\hbar}} |-a\rangle \sim e^{-\frac{S_E}{\hbar}} \sim e^{-\int_{-a}^{a} \frac{p(x)}{\hbar} dx} \ll 1 \tag{4.13}$$

We recover in this result the expected semiclassical tunneling coefficient.

For the specific example of a quartic potential $V(x) = \frac{\lambda}{4!}\left(x^2 - a^2\right)^2$, the zero energy solution satisfies

$$\dot{x} = \pm\frac{\omega}{2a}\left(x^2 - a^2\right) \tag{4.14}$$

where we used the new variable $\omega^2 = \frac{\lambda a^2}{3m}$.

The solutions of these equations are the instanton and anti-instanton given by

$$x(\tau) = \pm a \tanh\left(\frac{\omega}{2}(\tau - \tau_0)\right) \tag{4.15}$$

The instanton (with the plus sign) is depicted in figure 4.5.

Remarks

- For the instanton solution, the value of the exponent $\frac{S_E}{\hbar}$ is given by:

$$\frac{S_E}{\hbar} = \int_{-a}^{a} \frac{\sqrt{2mV(x)}}{\hbar} dx = \frac{2}{3}\sqrt{\frac{\lambda m}{3}}\frac{a^3}{\hbar}$$

$$= \frac{2}{3^{3/2}}\sqrt{\lambda m}\left(\frac{3m}{\lambda}\right)^{3/2}\frac{\omega^3}{\hbar} = 2\frac{m^2\omega^3}{\hbar\lambda} = \frac{2}{\bar{\lambda}} \tag{4.16}$$

where $\bar{\lambda} = \frac{\hbar\lambda}{m^2\omega^3}$ is the dimensionless parameter that characterizes the size of the perturbative corrections to the harmonic oscillator value for
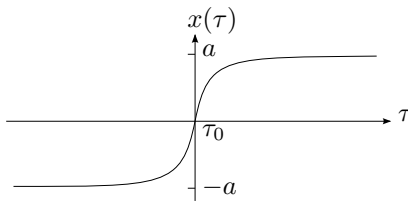
Figure 4.5: The instanton solution in the double well potential, running from $-a$ to a.

the energy levels. We already encountered $\bar{\lambda}$ when we studied perturbative corrections to the ground state energy of the harmonic oscillator with a λx^4 perturbation. Since Feynman diagrams with k-loops contribute a correction of order $\bar{\lambda}^{k-1}$, the coupling $\bar{\lambda}$ is often called a *loop-expansion parameter*.

The part of the Euclidean propagator due to the instantons is therefore proportional to $e^{-S_E/\hbar} = e^{-2/\bar{\lambda}}$. Thus, effects associated with instantons are non-perturbative in $\bar{\lambda}$.

- At $|\tau - \tau_0| \gtrsim \frac{1}{\omega}$, we have that $\left|x^2(\tau) - a^2\right| \approx e^{-\omega|\tau-\tau_0|} \ll 1$. Instantons are thus well localized in Euclidean time: they exist for a short instant $\Delta\tau \sim \frac{1}{\omega}$ in Euclidean time (hence their name).

Thus, when $\beta \to \infty$, up to exponentially small terms, we have $x \approx \pm a$ away from $\tau = \tau_0$. This is a crucial property considering that we are interested in the limit $\beta \to \infty$: for $\beta \gg \frac{1}{\omega}$ the instanton solution looks like a step function (see figure 4.6).
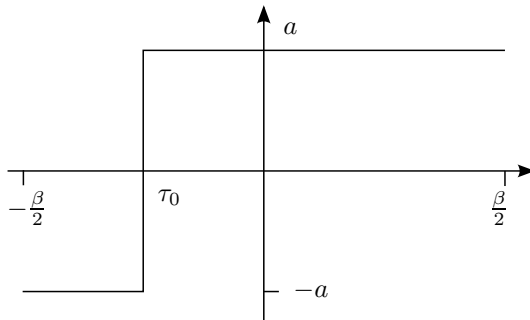

Figure 4.6: In the large β limit, the instanton solution looks like a step function.

After having jumped from $-a$ to a, there is still plenty of time to bounce back!

More technically, given the instanton solution $x_I(\tau) = af(\tau - \tau_0)$, where $|f(\tau - \tau_0)| = 1 - e^{-\omega|\tau-\tau_0|}$ for $|\tau - \tau_0| \gg \frac{1}{\omega}$, then

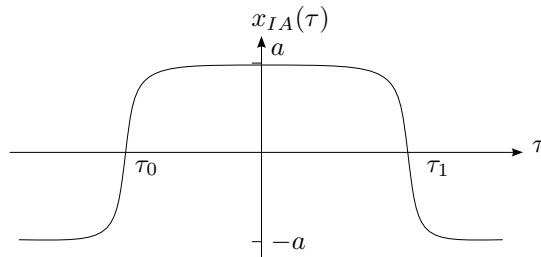$$x_{IA}(\tau) = af(\tau - \tau_0)f(\tau_1 - \tau) \tag{4.17}$$

Figure 4.7: The instanton-anti-instanton quasisolution.

for $\tau_1 \gg \tau_0$ is an <u>approximate</u> solution representing an instanton followed by an anti-instanton. For such a configuration, one can easily check that

$$\left.\frac{\delta S_E}{\delta x}\right|_{x=x_{IA}} \sim e^{-\omega|\tau_0 - \tau_1|} . \tag{4.18}$$

As long as we only need to consider situations where $\omega|\tau_0 - \tau_1|$ is so large that the above exponential is smaller than any effect we are trying to compute, then we should by all means consider the configuration x_{IA} as a stationary point of the action. And thus add the contribution of these quasi-solutions to our semiclassical approximation to the path integral. Indeed, we shall find at the end that $|\tau_1 - \tau_0| \sim e^{\frac{S_E}{\hbar}}$. Thus, neglecting that x_{IA} is not an exact solution amounts to neglecting terms of order $\mathcal{O}\left(e^{-\omega \exp(S_E/\hbar)}\right)$! These terms do not exactly vanish but are indeed very small. Thus we must add the contribution of x_{IA} to our saddle point estimate of the path integral.

- By extending this argument, we are easily convinced that we must consider all the approximate solutions with a number N of instantons + anti-instantons. Notice that if we take n_I instantons and n_A anti-instantons, we must have that $n_I - n_A = 0$ for $a \to a$, and $n_I - n_A = 1$ for $-a \to a$. (what about $-a \to -a$ and $a \to -a$?)

  An approximate solution with, e.g. three instantons at τ_1, τ_3 and τ_5 and two anti-instantons at τ_2 and τ_4 will be a good one provided $\tau_1 \ll \tau_2 \ll \tau_3 \ll \tau_4 \ll \tau_5$. We will check later whether this condition is satisfied for the leading terms.

4.2.1 The multi-instanton amplitude

We will now compute our amplitudes by summing over all possible sequences of widely separated instantons (and anti-instantons): this is the <u>diluted instanton gas approximation</u>.

Each of these quasi-solutions contributes to the amplitude in two ways:

Exponent: the contribution to S_E is localized at each instanton (or anti-instanton) transition time. Indeed, away from these transition times, the quasi-solution is close to $\pm a$ with a neglectible velocity. S_E is therefore zero in these regions.
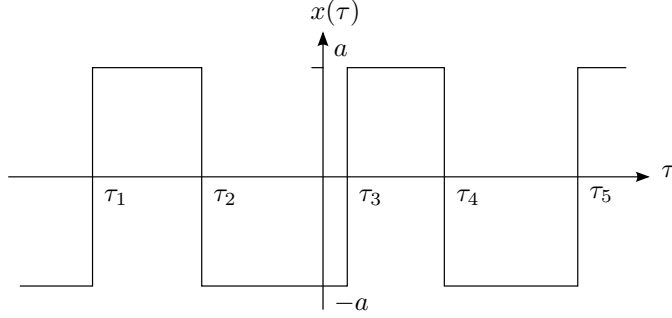
Figure 4.8: A quasi-solution with three instantons localized at τ_1, τ_3 and τ_5, and two anti-instantons localizd at τ_2 and τ_4.

Each instanton (or anti-instanton) will give a factor S_I in the action. Due to the decomposition property of the action, the contribution of an approximate solution with N instantons and anti-instantons will be:

$$S_N = NS_I \quad \Rightarrow \quad e^{-\frac{S_N}{\hbar}} = e^{-N\frac{S_I}{\hbar}} \tag{4.19}$$

Determinant prefactor: notice again that away from the very short <u>instants</u> over which the transitions take place, the system sits at either one of its classical vacua at $x = \pm a$, around which $V''(x) = \frac{m\omega^2}{2}$.

If we had $V''(\bar{x}) \equiv \frac{m\omega^2}{2}$ throughout the interval $\left[-\frac{\beta}{2}, \frac{\beta}{2}\right]$, then the prefactor would be the usual one for the harmonic oscillator:

$$\tilde{\mathcal{N}} \left(\det \left(-m\frac{d^2}{d\tau^2} + V''(\bar{x}) \right) \right)^{-\frac{1}{2}} = \left(\frac{m\omega}{2\pi\hbar \sinh(\omega\beta)} \right)^{\frac{1}{2}} \approx \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} e^{-\frac{\omega\beta}{2}}$$

Given the factorization property of the path integral and, in particular, of the Gaussian integral we are interested in, we expect that each transition will correct the prefactor of the harmonic oscillator with a factor R.

We thus expect

$$\begin{cases} \tilde{\mathcal{N}} \left(\det \left(-m\frac{d^2}{d\tau^2} + V''(\bar{x}) \right) \right)^{-\frac{1}{2}} = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} e^{-\frac{\omega\beta}{2}} R^n \\ n = n_I + n_A \end{cases} \tag{4.20}$$

for a quasi-solution with n instantons and anti-instantons.

Let us see how this argument can be made sharper, by focussing on the simplest non-trivial case of an x_{IA} solution. (The generalization to an arbitrary sequence of I and A is straightforward.) To do so, we explicitly write the Gaussian integral in factorized form by considering intermediate times around instanton $\tau_1^\pm = \tau_1 \pm \Delta$ and around anti-instanton $\tau_2^\pm = \tau_2 \pm \Delta$ as shown in figure. We define the integration coordinates at intermediate times as $x(\tau_i^\pm) = x_i^\pm$, for $i = 1, 2$. The Euclidean propagator can thus be
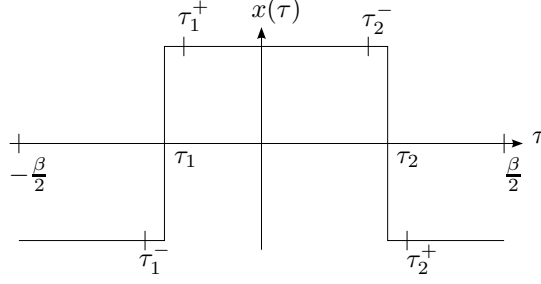
Figure 4.9: Intermediate times $\tau_i^{\pm} = \tau_i \pm \Delta$ have been added to the instanton-anti-instanton quasisolution, with $|\tau_i - \tau_j| \gg \Delta \gg \frac{1}{\omega}$, so that at $\tau_i^{\pm}$, the solution is almost in the vacuum.

factorized into the convolution of the propagator over five time intervals (see figure)

$$K_E(-a, -a; \frac{\beta}{2}, -\frac{\beta}{2}) = \int dx_1^- dx_1^+ dx_2^- dx_2^+ \underbrace{K_E(-a, x_2^+; \frac{\beta}{2}, \tau_2^+)}_{(1)} \times$$

$$K_E(x_2^+, x_2^-; \tau_2^+, \tau_2^-) \underbrace{K_E(x_2^-, x_1^+; \tau_2^-, \tau_1^+)}_{(2)} \times$$

$$K_E(x_1^+, x_1^-; \tau_1^+, \tau_1^-) \underbrace{K_E(x_1^-, -a; \tau_1^-, -\frac{\beta}{2})}_{(3)} \quad (4.21)$$

Of course we work under the assumption $|\tau_2 - \tau_1| \gg \frac{1}{\omega}$. The factorization turns out to be useful if we also choose $\Delta \gg \frac{1}{\omega}$. Indeed it is intuitively clear that, for $\omega\Delta \gg 1$, the amplitudes (1), (2) and (3) should be well approximated (exponentially well indeed!) by harmonic oscillator amplitudes. This is because, during the corresponding time intervals, the trajectory sits very close to one or the other minimum, where the potential is well approximated by the harmonic oscillator one. Moreover, we know that the harmonic oscillator amplitude, for large euclidean time separation, is dominated by the ground state (see section 2.3). We can thus approximate, e.g. amplitude (2), by:

$$\begin{aligned} K_E(x_2^-, x_1^+; \tau_2^-, \tau_1^+) &= \langle x_2^- | e^{-\frac{H_0}{\hbar}(\tau_2^- - \tau_1^+)} | x_1^+ \rangle \left(1 + O(e^{-\omega\Delta})\right) \\ &\approx \langle 0_+ | e^{-\frac{H_0}{\hbar}(\tau_2^- - \tau_1^+)} | 0_+ \rangle \, \Psi_0^{+\,*}(x_2^-) \Psi_0^+(x_1^+) \\ &= \Psi_0^{+\,*}(x_2^-) \Psi_0^+(x_1^+) e^{-\frac{\omega}{2}(\tau_2^- - \tau_1^+)} \end{aligned} \quad (4.22)$$

where H_0 represent the harmonic oscillator Hamiltonian around $+a$. Here we also decomposed position eigenvectors $|x\rangle$ into eigenstates of the harmonic oscillator Hamiltonian around $+a$: $|x\rangle = \sum_{n_+} \Psi_n^+(x) |n_+\rangle$, and we kept only the ground state contribution.

By applying the same approximation to (1) and (3) as well, and expanding into the similarly defined harmonic oscillators eigenstates around $-a$, we

can thus write the Euclidean propagator as

$$K_E(-a, -a; \frac{\beta}{2}, -\frac{\beta}{2}) \approx \int dx_1^- dx_1^+ dx_2^- dx_2^+ \left| \Psi_0^-(-a) \right|^2 e^{-\frac{\omega\beta}{2}}$$

$$\Psi_0^-(x_2^+) \, \Psi_0^{+\,*}(x_2^-) \Psi_0^+(x_1^+) \, \Psi_0^{-\,*}(x_1^-) e^{\frac{\omega}{2}((\tau_2^+ - \tau_2^-) + (\tau_1^+ - \tau_1^-))}$$

$$K_E(x_2^+, x_2^-; \tau_2^+, \tau_2^-) K_E(x_1^+, x_1^-; \tau_1^+, \tau_1^-)$$

$$= \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} e^{-\frac{\omega\beta}{2}} R^2 \tag{4.23}$$

where

$$R = \int dx_1^- dx_1^+ e^{\frac{\omega}{2}(\tau_1^+ - \tau_1^-)} \Psi_0^+(x_1^+) \, \Psi_0^{-\,*}(x_1^-) K_E(x_1^+, x_1^-; \tau_1^+, \tau_1^-) \tag{4.24}$$

R will be fixed later on by studying more carefully the one-instanton amplitude. This proves factorization as promised.

We are not done yet!

We must still sum over over the locations $\tau_1, \ldots, \tau_n$ of the instantons. Indeed, as long as $\tau_1 \ll \tau_2 \ll \cdots \ll \tau_n$, we still get an equally good approximate solution by moving the positions τ_i around. The summation over instanton and anti-instanton location simply (and obviously) corresponds to the integral:

$$\int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau_n \int_{-\frac{\beta}{2}}^{\tau_n} d\tau_{n-1} \cdots \int_{-\frac{\beta}{2}}^{\tau_2} d\tau_1 = \frac{\beta^n}{n!} \tag{4.25}$$

How do we normalize the $d\tau_i$ integrals? This is not a problem for the moment: the normalization can be absorbed by the factor R (and this is not by chance!).

Finally, one thing we have to be careful about is that instantons and anti-instantons cannot be distributed arbitrarily: for example, starting at $-a$ we must first encounter an instanton. For $\langle -a | e^{-\frac{\beta H}{\hbar}} | -a \rangle$, all contributions will have $n_I = n_A$, etc...

We can now put together all the pieces and compute the total <u>semiclassical</u> amplitudes.

4.2.2   Summing up the instanton contributions: results

Let us compute $\langle -a | e^{-\frac{\beta H}{\hbar}} | -a \rangle$ first. The contributing solutions are depicted in figure 4.10.
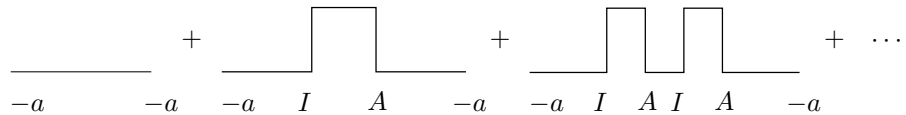

Figure 4.10: The contributing solutions for the tranition from $-a$ to $-a$ are solutions with any number of instanton-anti-instanton pairs.

Thus, the amplitude will be:

$$\langle -a | e^{-\frac{\beta H}{\hbar}} | -a \rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} e^{-\frac{\beta\omega}{2}} \cdot \sum_{n=\text{even}} \frac{\left(Re^{-S_I/\hbar}\beta \right)^n}{n!} \cdot [1 + \mathcal{O}(\hbar)] \quad (4.26)$$

Similarly, we can compute $\langle a | e^{-\frac{\beta H}{\hbar}} | -a \rangle$:

$$\langle a | e^{-\frac{\beta H}{\hbar}} | -a \rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} e^{-\frac{\beta\omega}{2}} \cdot \sum_{n=\text{odd}} \frac{\left(Re^{-S_I/\hbar}\beta \right)^n}{n!} \cdot [1 + \mathcal{O}(\hbar)] \quad (4.27)$$

Performing the summation, we get:

$$\langle \pm a | e^{-\frac{\beta H}{\hbar}} | -a \rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} e^{-\frac{\beta\omega}{2}} \cdot \frac{1}{2} \left(e^{Re^{-S_I/\hbar}\beta} \mp e^{-Re^{-S_I/\hbar}\beta} \right) \cdot [1 + \mathcal{O}(\hbar)]$$
$$(4.28)$$

Recalling that

$$\langle x_f | e^{-\frac{\beta H}{\hbar}} | x_i \rangle = \sum_n \Psi_n^*(x_f) \Psi_n(x_i) e^{-\frac{\beta E_n}{\hbar}} \quad (4.29)$$

and comparing to (4.28), we can read out (for $\beta \to \infty$) the energies of the lowest energy states:

$$E_\pm = \frac{\hbar\omega}{2} \pm \hbar R e^{-\frac{S_I}{\hbar}} \quad (4.30)$$

Calling $|+\rangle$ and $|-\rangle$ the corresponding eigenstates, we can write

$$\langle \pm a | e^{-\frac{\beta H}{\hbar}} | -a \rangle = \Psi_+^*(\pm a)\Psi_+(-a) e^{-\frac{\beta E_+}{\hbar}} + \Psi_-^*(\pm a)\Psi_-(-a) e^{-\frac{\beta E_-}{\hbar}} \quad (4.31)$$

Comparing to (4.28), and calling

$$\psi_0(x) \equiv \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} \quad (4.32)$$

the harmonic oscillator ground state wavefunction we get

$$\Psi_-^*(\pm a)\Psi_-(-a) = \frac{1}{2} \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} = \left(\frac{1}{\sqrt{2}} \psi_0(0) \right)^2$$

$$\Psi_+^*(\pm a)\Psi_+(-a) = \mp \frac{1}{2} \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} = \mp \left(\frac{1}{\sqrt{2}} \psi_0(0) \right)^2$$

$$\Rightarrow \begin{cases} \Psi_-(x) \text{ is even} & \Psi_-(a) = \Psi_-(-a) \\ \Psi_+(x) \text{ is odd} & \Psi_+(a) = -\Psi_+(-a) \end{cases} \quad (4.33)$$

as expected from the usual Schrödinger approach.

Basically,

$$\Psi_\pm(x) = \frac{1}{\sqrt{2}} \left(\psi_0(x + a) \mp \psi_0(x - a) \right)$$

Let us now add a few comments about our results.

1. Notice that in our computation, we have neglected the <u>perturbative</u> corrections.

   Technically speaking, equation (4.30) is "incorrect" because in it, we have only retained the instanton correction which is of order

   $$\hbar e^{-S/\hbar} \sim \hbar e^{-2/\bar{\lambda}} \tag{4.34}$$

   and is smaller than the perturbative corrections (!) we previously computed by Feynman diagrams:

   $$\Delta E_n \sim \hbar \omega \bar{\lambda}^n \tag{4.35}$$

   The point, however, is that these perturbative correction affect E_+ and E_- by <u>exactly</u> the same amount: they cancel in $E_+ - E_-$.

   A purist (as Coleman puts it) would only retain the instanton contribution when writing the difference

   $$E_+ - E_- = 2\hbar R e^{-S_I/\hbar} = 2\hbar R e^{-2/\bar{\lambda}} \tag{4.36}$$

   One could go ahead and compute the perturbative corrections to $\langle \pm a | e^{-\frac{\beta H}{\hbar}} | -a \rangle$ with the same Feynman diagram techniques we used before; we would have to compute the Green's function around each solution.

   For most of the time, the instanton solutions sit at either one or the other minimum. The perturbative corrections are thus the same as those we have computed before, plus corrections coming from the cubic anharmonic term (see figure 4.11).
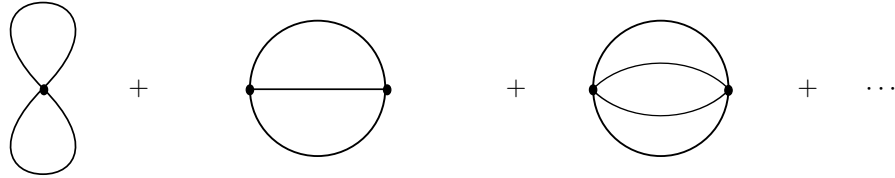

Figure 4.11: The quantum corrections to the classical solutions. The first diagram is a two-loop correction involving the $\lambda_4 x^4$ correction, the second one is a two-loop correction involving the $\lambda_3 x^3$ correction, and the third one is a three-loop correction.

For instance, $\langle a | e^{-\frac{\beta H}{\hbar}} | -a \rangle$ becomes:

$$\langle a | e^{-\frac{\beta H}{\hbar}} | -a \rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} e^{-\frac{\beta E_0(\lambda)}{\hbar}} \sum_{n=\text{odd}} \frac{\left(R(\lambda) e^{-S_I/\hbar} \beta \right)^n}{n!}$$

$$E_0(\lambda) = \frac{\hbar\omega}{2} \left(1 + \sum_{n=1}^{\infty} c_n \bar{\lambda}^n \right)$$

$$R(\lambda) = R \left(1 + \sum_{n=1}^{\infty} d_n \bar{\lambda}^n \right) \tag{4.37}$$

where c_n are the loop coefficient we have computed previously, and R is the leading contribution to the prefactor we introduced before without computing it explicitly.

Moral: we see the two classes of effects at work:

- Non-perturbative effects, determined by semiclassical methods. They correspond to the <u>non-trivial</u> stationary points of the Euclidean action.

- Perturbative effects. They correspond to <u>small</u> quantum fluctuations around each stationary point of the action: they are the functional integral analogue of the corrections to the saddle point approximation of ordinary integrals. The perturbative corrections are conveniently organized in a series of Feynman diagrams.

  The leading $\mathcal{O}\left(\bar{\lambda}^0\right)$ term corresponds to evaluating the quantum fluctuation determinant $\frac{1}{\sqrt{\det(\hat{O})}}$.

  - $\mathcal{O}\left(\bar{\lambda}\right)$ terms correspond to two-loops diagrams.
  - $\mathcal{O}\left(\bar{\lambda}^2\right)$ terms correspond to three-loops diagrams.
  - And so on. . .

2. We can now also check the validity of our dilute instanton approximation.

   The exponential series $\sum \frac{(Re^{-S_I/\hbar}\beta)^n}{n!}$ is dominated by the terms with $n \sim Re^{-S_I/\hbar}\beta$. Thus, the typical instanton density is: $\rho \approx \frac{n}{\beta} = Re^{-S_I/\hbar}$. It is exponentially small! Their average separation in time is:

   $$\Delta\tau = \frac{1}{\rho} = \frac{e^{S_I/\hbar}}{R} = \frac{1}{\Delta E} \tag{4.38}$$

   which is <u>independent of β</u>.

   The sum over the instantons is truly necessary only to reproduce the exponential behaviour of $\left\langle e^{\frac{-\beta H}{\hbar}} \right\rangle$ at $\beta > \frac{1}{\Delta E}$.

   We can now go back and verify that the sequences of widely separated instanton anti-instanton that are relevant to our result are stationary points of the action up to effects of order

   $$\left.\frac{\delta S}{\delta x}\right|_{x=x_{IA}} \sim e^{-\omega|\tau_1-\tau_2|} \approx e^{-\left[\frac{\omega}{R}e^{S_I/\hbar}\right]} \tag{4.39}$$

   which is truly small! Much-much smaller than the $e^{-2/\bar{\lambda}}$ effects we have been computing.

3. Another puzzle that one could have pointed out when we started our computation concerned the relevance of multi-instanton trajectories. These have an euclidean action $= nS_I$ which is bigger that the single instanton one S_I. The contribution of each such trajectory is thus weighted by a much smaller exponential factor, and one may wonder if it makes any sense to include them at all. For instance in $\langle +a|e^{-\beta H}|-a\rangle$ a IAI configuration contributes with weight e^{-3S_I}, which is exponentially smaller than the one instanton contribution e^{-S_I}. Now, at the end of our computation,

we obviously know how to answer. Each multi-instanton contributes only $\propto e^{-nS_I}$ to the amplitude, however n-instantons have also a higher multiplicity $\propto R^n \beta^n / n!$ which for $R\beta > e^{-S_I}$ compensates for the exponential suppression. We can here draw a simple statistical mechanics analogy (just an analogy!): the action exponent plays the role of Boltzmann factor $\propto e^{-nS_I} \sim e^{-E/T}$, the multiplicity $\propto R^n \beta^n / n$ plays the role of an entropy factor e^S, while the amplitude we are computing is the analogue of the partition function $e^{-F/T}$. Boltzmann suppressed configurations contribute significantly to the free energy at equilibrium if they have large multiplicity.

4.2.3 Cleaning up details: the zero-mode and the computation of R

To wrap things up, we are left with explaining the origin of the $d\tau$ integral on the instanton position and with computing R (the two things are obviously related).

We have to study $\det \left(\frac{\delta^2 S}{\delta x^2} \right)\Big|_{x=x_I}$, the fluctuation determinant around the one-instanton solution.

Surprise:

$$\frac{\delta^2 S}{\delta x^2}\bigg|_{x=x_I} = -m\partial_\tau{}^2 + V_E''(x_I) \tag{4.40}$$

possesses one normalizable zero mode:

$$\begin{cases} \left(-m\partial_\tau{}^2 + V_E''(x_I)\right) y_0(\tau) = 0 \\[2mm] \displaystyle\int_{-\infty}^{\infty} |y_0(\tau)|^2 \, d\tau = 1 \end{cases} \tag{4.41}$$

Indeed, we can compute from the equation of motion:

$$-m\partial_\tau{}^2 x_I(\tau) + V_E'(x_I(\tau)) = 0$$
$$\Rightarrow \quad -m\partial_\tau{}^2 \dot{x}_I(\tau) + V_E''(x_I(\tau))\dot{x}_I(\tau) = 0 \tag{4.42}$$

We can then compute the normalization of this zero mode:

$$\int \dot{x}_I{}^2(\tau)d\tau = \frac{1}{m} \int m\dot{x}_I{}^2(\tau)d\tau = \frac{S_I}{m}$$
$$\Rightarrow \quad y_0(\tau) = \sqrt{\frac{m}{S_I}} \dot{x}_I(\tau) \tag{4.43}$$

The presence of Ψ_0 originates from the invariance of the action under time translations: $x_I(\tau + \Delta) = x_I^\Delta$ is a solution with same boundary conditions as $x_I(\tau)$, $\forall \Delta \in \mathbb{R}$, which implies that $S(x_I) = S(x_I^\Delta)$. Thus, $\frac{\delta^2 S}{\delta x^2} = 0$ along this direction in the function space.

We can now expand the function x into modes around $x_I{}^2$:

$$x(\tau) = x_I(\tau) + \sqrt{\hbar} \underbrace{\sum_n y_n(\tau)\tilde{a}_n}_{y(\tau)} \tag{4.44}$$

---

[2]We are using the same normalization of section 3.1

Thus,

$$\exp\left(-\frac{1}{2\hbar}\frac{\delta^2 S}{\delta x^2}y^2\right) = \exp\left(-\frac{1}{2}\sum_n \lambda_n \tilde{a}_n{}^2\right) = \exp\left(-\frac{1}{2}\lambda_1\tilde{a}_1{}^2 - \frac{1}{2}\lambda_2\tilde{a}_2{}^2 + \cdots\right) \tag{4.45}$$

as $\lambda_0 = 0$.

The integration over $\tilde{a}_0$ should be treated separately and with special care (otherwise we would get a $\frac{1}{\lambda_0}$ nonsense).

Notice that $d\tilde{a}_0$ is associated to a shift in the time position of the instanton:

$$x(\tau) = x_I(\tau) + \sqrt{\frac{\hbar m}{S_I}}\dot{x}_I(\tau)\cdot\tilde{a}_0 + \cdots \approx x_I\left(\tau + \tilde{a}_0\sqrt{\frac{\hbar m}{S_I}}\right) + \cdots$$

$$x_I(\tau) = f(\tau - \tau_0) \quad\Rightarrow\quad \sqrt{\frac{\hbar m}{S_I}}d\tilde{a}_0 = -d\tau_0 \tag{4.46}$$

Let us then choose an N such that the measure for the fluctuation $y(\tau)$ is:

$$\mathscr{D}[y] = \tilde{\mathcal{N}}\prod_n \frac{d\tilde{a}_n}{\sqrt{2\pi}} \tag{4.47}$$

N is fixed as usual by some simple reference system; for example the harmonic oscillator:

$$S_E = \frac{m\dot{y}^2}{2} + \frac{m\omega^2 y^2}{2} \quad\rightarrow\quad \lambda_n^h(\omega) = m\left[(\frac{\pi n}{\beta})^2 + \omega^2\right] \tag{4.48}$$

$$\tilde{\mathcal{N}}\int\prod_n \frac{d\tilde{a}_n}{\sqrt{2\pi}}e^{-\frac{1}{2}\sum_n \lambda_n^h \tilde{a}_n{}^2} = \tilde{\mathcal{N}}\left(\prod_n \lambda_n^h\right)^{-\frac{1}{2}} =$$

$$\sqrt{\frac{m\omega}{2\pi\hbar\sinh(\beta\omega)}} = \frac{\tilde{\mathcal{N}}}{\sqrt{\det\left(-m\partial_\tau{}^2 + m\omega^2\right)}} \tag{4.49}$$

Let us now integrate in our case by separating out the integral on the zero mode. We have

$$\tilde{\mathcal{N}}\int\prod_n \frac{d\tilde{a}_n}{\sqrt{2\pi}}e^{-\frac{1}{2}\sum_n \lambda_n \tilde{a}_n{}^2} = \int d\tau_0 \sqrt{\frac{S_I}{m\pi\hbar}}\cdot\tilde{\mathcal{N}}\prod_{n\geq 1}\frac{d\tilde{a}_n}{\sqrt{2\pi}}e^{-\frac{1}{2}\sum_n \lambda_n \tilde{a}_n{}^2}$$

$$= \int d\tau_0 \sqrt{\frac{S_I}{m\pi\hbar}}\cdot\frac{\tilde{\mathcal{N}}}{\sqrt{\det\left(-m\partial_\tau{}^2 + m\omega^2\right)}}\cdot\frac{\sqrt{\det\left(-m\partial_\tau{}^2 + m\omega^2\right)}}{\sqrt{\det'\left(-m\partial_\tau{}^2 + V''(x_I)\right)}}$$

$$= \int d\tau_0 \sqrt{\frac{S_I}{m\pi\hbar}}\cdot\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}}e^{-\frac{\beta\omega}{2}}\cdot\sqrt{\frac{\det\left(-m\partial_\tau{}^2 + m\omega^2\right)}{\det'\left(-m\partial_\tau{}^2 + V''(x_I)\right)}} \tag{4.50}$$

where we multiplied and divided by the harmonic oscillator determinant, used eq. (4.49) and took the $\beta\omega \gg 1$ limit. By $\det'$ we indicate the determinant with the zero mode removed: $\det' = \lambda_1\cdot\lambda_2\cdot\lambda_3\cdot\ldots$. Now, by a straightforward but tedious computation which we shall not do explicitly [3] one finds

$$\sqrt{\frac{S_I}{m\pi\hbar}}\sqrt{\frac{\det\left(-m\partial_\tau{}^2 + m\omega^2\right)}{\det'\left(-m\partial_\tau{}^2 + V''(x_I)\right)}} = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}}\tilde{v} \equiv R \tag{4.51}$$

[3]To be found in Coleman's lectures and also proposed in one of the Homeworks to be posted on line (next year...).

where $\tilde{v}$ is determined by the asymptotic behaviour of $\dot{x}_I$ for $|\tau - \tau_0| \gg \frac{1}{\omega}$:

$$\dot{x}_I = \tilde{v}e^{-\omega|\tau - \tau_0|} \tag{4.52}$$

In the specific case of the $\frac{\lambda}{4!}\left(x^2 - a^2\right)^2$ potential, we have:

$$x(\tau) = a\frac{1 - e^{-\omega(\tau - \tau_0)}}{1 + e^{-\omega(\tau - \tau_0)}} \overset{\tau - \tau_0 \gg \frac{1}{\omega}}{\longrightarrow} a\left(1 - 2e^{-\omega(\tau - \tau_0)}\right)$$

$$\Rightarrow \quad \dot{x} \overset{\tau - \tau_0 \gg \frac{1}{\omega}}{\longrightarrow} 2a\omega e^{-\omega|\tau - \tau_0|}$$

$$\Rightarrow \quad \tilde{v} = 2a\omega \tag{4.53}$$

Thus, we can compute:

$$\left(\frac{m\omega}{\pi\hbar}\tilde{v}^2\right)^{\frac{1}{2}} = \left(\frac{4ma^2\omega^3}{\pi\hbar}\right)^{\frac{1}{2}} = \left(\frac{12m^2\omega^5}{\pi\hbar\lambda}\right)^{\frac{1}{2}} = \left(\frac{12}{\pi\lambda}\right)^{\frac{1}{2}}\omega \tag{4.54}$$

We thus finally obtain the energy splitting between the two lowest energy levels:

$$E_+ - E_- = 2\hbar\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}}\tilde{v}e^{-\frac{S_I}{\hbar}} \tag{4.55}$$

Chapter 5

Interaction with an external electromagnetic field

We will now discuss the quantum mechanics of a particle interacting with an external electromagnetic field. We will see that the path integral approach offers a neat viewpoint on the issue of gauge invariance and on the role of topology.

5.1 Gauge freedom

5.1.1 Classical physics

The relativistically invariant action for a neutral spinless particle is

$$S = -mc^2 \int_\gamma d\tau = -mc^2 \int_\gamma \sqrt{1 - \frac{\dot{x}^2}{c^2}} dt \qquad (5.1)$$

where we have chosen the parametrization so that:

$$\begin{cases} d\tau^2 = (dx^0)^2 - \dfrac{1}{c^2}(dx^i)^2 = \left[(\partial_\sigma x^0)^2 - \dfrac{1}{c^2}(\partial_\sigma x^i)^2\right] d\sigma^2 \\[2ex] \sigma = x^0 \equiv t \ \Rightarrow \ d\tau = \sqrt{1 - \dfrac{\dot{x}^2}{c^2}} dt \end{cases} \qquad (5.2)$$

The simplest relativistic invariant interaction with the electromagnetic quadrivector field $A_\mu = (A_0, -A^i)$ is obtained by modifying eq. (5.1) to

$$S = -mc^2 \int_\gamma d\tau - e \int_\gamma A_\mu dx^\mu = -\int_\gamma \left[mc^2 \sqrt{1 - \frac{\dot{x}^2}{c^2}} + eA_0 - eA^i \dot{x}^i \right] dt \quad (5.3)$$

The coefficient e is the electric charge of the particle.

Notice that the gauge transformation $A_\mu \to A_\mu + \partial_\mu \alpha$ does not affect the equations of motion since S only changes by boundary terms.

$$S \to S - e\left(\alpha(x_f, t_f) - \alpha(x_i, t_i)\right)$$

Consequently the classical equations of motion only depend on the electromagnetic fields $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, which are local functions of A_μ that are not affected by gauge transformations.

The classically relevant quantity is the electromagnetic field $F_{\mu\nu}$, but the lagrangian involves a <u>redundant</u> quantity: A_μ.

Let us consider now what happens in the Hamiltonian description of this system.

From equation (5.3), we can find the conjugate momenta:

$$p^i = \frac{\partial \mathcal{L}}{\partial \dot{x}^i} = \frac{m\dot{x}^i}{\sqrt{1 - \frac{\dot{x}^2}{c^2}}} + eA^i(x,t) \tag{5.4}$$

This leads to the hamiltonian:

$$H = p^i \dot{x}^i - \mathcal{L} = \sqrt{(p^i - eA^i)^2 c^2 + m^2 c^4} + eA_0 \tag{5.5}$$

where $A_0 = V$ is the electromagnetic potential.

Remark: both p^i and H are <u>not</u> invariant under a change of gauge for A_μ:

$$\begin{cases} p^i = \dfrac{m\dot{x}^i}{\sqrt{1 - \frac{\dot{x}^2}{c^2}}} + eA^i(x,t) & \rightarrow p'^i = p^i - e\partial_i\alpha \\[4mm] H = \sqrt{(p^i - eA^i)^2 c^2 + m^2 c^4} + eA_0 & \rightarrow H' = H + e\partial_0\alpha \end{cases} \tag{5.6}$$

(H, p^i) transforms like $e(A_0, A^i)$.

Notice that the kinetic momentum is gauge invariant (being just a function of the velocity):

$$\Pi^i \equiv \frac{m\dot{x}^i}{\sqrt{1 - \frac{\dot{x}^2}{c^2}}} = p^i - eA^i \;\rightarrow\; \left(p^i - e\partial_i\alpha\right) - e\left(A^i - \partial_i\alpha\right) = \Pi^i \tag{5.7}$$

Now what is the transformation (5.6) in the Hamiltonian language? Defining $F(x,t) \equiv e\alpha$, we can write:

$$\begin{cases} p^i \rightarrow p'^i = p^i - \partial_i F \\ x^i \rightarrow x'^i = x^i \\ H(p,x) \rightarrow H'(p',x') = H(p,x) + \partial_0 F \end{cases} \tag{5.8}$$

It is a <u>canonical transformation</u>, in the sense that the following relations are satisfied:

$$\left\{p'^i, p'^j\right\} = \frac{\partial p'^i}{\partial p^k}\frac{\partial p'^j}{\partial x^k} - \frac{\partial p'^i}{\partial x^k}\frac{\partial p'^j}{\partial p^k} = \delta_{ik}(-\partial_{kj}F) - (-\partial_{jk}F)\delta_{ik} = 0$$

$$\left\{p'^i, x'^j\right\} = \frac{\partial p'^i}{\partial p^k}\frac{\partial x'^j}{\partial x^k} - \frac{\partial p'^i}{\partial x^k}\frac{\partial x'^j}{\partial p^k} = \delta_{ik}\delta_{jk} = \delta_{ij} \tag{5.9}$$

and, moreover, p'^i and x'^i satisfy the Hamilton equations for H':

$$\begin{cases} \dfrac{\partial p'^i}{\partial t} = \dfrac{\partial H'}{\partial x'^i} \\[3mm] \dfrac{\partial x'^i}{\partial t} = \dfrac{\partial H'}{\partial p'^i} \end{cases} \tag{5.10}$$

H and p^i are <u>not invariant</u> under gauge transformations, but they are <u>covariant</u>:

$$\left(H, p^i\right) \ \rightarrow \ \left(H, p^i\right) + e\left(\partial_0 \alpha, -\partial_i \alpha\right) \tag{5.11}$$

5.1.2 Quantum physics

Now, what happens to gauge invariance upon quantization? We will study the path integral viewpoint first, and the Hamiltonian viewpoint later.

In the path integral formalism, we can write very simply:

$$K(x_f, t_f; x_i, t_i) = \int \mathscr{D}[x] e^{\frac{iS[x]}{\hbar}}$$

$$\rightarrow \int \mathscr{D}[x] e^{\frac{iS[x]}{\hbar} - \frac{ie}{\hbar} \int_{x_i, t_i}^{x_f, t_f} d\alpha} = e^{-\frac{ie}{\hbar} \alpha(x_f, t_f)} K(x_f, t_f; x_i, t_i) e^{\frac{ie}{\hbar} \alpha(x_i, t_i)} \tag{5.12}$$

We have the relation:

$$\Psi(x_f, t_f) = \int K(x_f, t_f; x_i, t_i) \Psi(x_i, t_i) dx_i \tag{5.13}$$

The gauge covariance of this equation leads to:

$$\Psi(x, t) \ \rightarrow \ e^{-\frac{ie}{\hbar} \alpha(x, t)} \Psi(x, t) \tag{5.14}$$

This is what we should have expected!

Indeed, <u>classically</u>, the gauge transformation of the electromagnetic quadrivector field is related to a canonical transformation of the Hamiltonian variables:

$$\begin{cases} A_\mu \ \overset{\text{gauge}}{\underset{\text{transformation}}{\longrightarrow}} \ A_\mu + \partial_\mu \alpha \\ \left. \begin{matrix} x^i \\ p^i \\ H \end{matrix} \ \overset{}{\underset{\text{transformation}}{\overset{\text{canonical}}{\longrightarrow}}} \ \begin{cases} x^i \\ p^i - e\partial_i \alpha \\ H + e\partial_t \alpha \end{cases} \right. \end{cases} \tag{5.15}$$

<u>Quantum mechanically</u>, we can make an analogy with this representation:

$$\begin{cases} A_\mu \ \overset{\text{gauge}}{\underset{\text{transformation}}{\longrightarrow}} \ A_\mu + \partial_\mu \alpha \\ \Psi \ \overset{\text{canonical}}{\underset{\text{transformation}}{\longrightarrow}} \ e^{-\frac{ie}{\hbar} \alpha} \Psi \end{cases} \tag{5.16}$$

Indeed, $\Psi \rightarrow U\Psi$ with $U^\dagger U = UU^\dagger = \mathbb{1}$ is the most general canonical transformation in the quantum description. Under the above rotation of the state vectors, the matrix elements of any operator $\hat{O}$ transform like $\langle \Psi_1 | \hat{O} | \Psi_2 \rangle \rightarrow \langle \Psi_1 | U^\dagger \hat{O} U | \Psi_2 \rangle$. As the only thing that matters are matrix elements, very much like we do when going from the Schroedinger to the Heisenberg picture for time evolution, we could alternatively define the transformation as one where state vectors are unaffected while operators transform according to $\hat{O} \rightarrow U^\dagger \hat{O} U$. Canonical commutation relations are indeed preserved by the that transformation:

$$[\hat{p}, \hat{x}] = -i\hbar \mathbb{1} \ \rightarrow \ \left[U^\dagger \hat{p} U, U^\dagger \hat{x} U\right] = U^\dagger [\hat{p}, \hat{x}] U = -i\hbar U^\dagger U = -i\hbar \mathbb{1} \, . \tag{5.17}$$

These results immediately tell us how to proceed in the Hamiltonian approach.

Let us quantize $p^i, x^j \to \hat{p}^i, \hat{x}^j$, with the canonical commutation relations:

$$[\hat{p}^i, \hat{p}^j] = [\hat{x}^i, \hat{x}^j] = 0$$
$$[\hat{p}^i, \hat{x}^j] = -i\hbar\delta_{ij} \tag{5.18}$$

In the non-relativistic limit where $\frac{\dot{x}}{c} \ll 1$, the classical Hamiltonian takes the form:

$$H = mc^2 + \frac{1}{2m}\left(p^i - eA^i\right)^2 + eA_0. \tag{5.19}$$

Quantizing and neglecting the (now irrelevant) constant mc^2 we have the Hamiltonian operator

$$H(\hat{p}, \hat{x}) = \frac{1}{2m}\left(\hat{p}^i - eA^i(\hat{x})\right)^2 + eA_0(\hat{x}) \tag{5.20}$$

Let us now work in the coordinate representation, where

$$\hat{x}^i = x^i \qquad \hat{p}^i = -i\hbar\frac{\partial}{\partial x^i} \tag{5.21}$$

The matrix elements of $\hat{p}^i$ are not invariant under the gauge transformation $\Psi \to e^{-\frac{ie}{\hbar}\alpha}\Psi$:

$$\langle\Psi_1|\,\hat{p}^j\,|\Psi_2\rangle = \int d^3x\Psi_1^*(x)(-i\hbar\partial_j)\Psi_2(x)$$

$$\to \int d^3x\Psi_1^* e^{\frac{ie}{\hbar}\alpha}(-i\hbar\partial_j)e^{-\frac{ie}{\hbar}\alpha}\Psi_2 = \int d^3x\Psi_1^*(-i\hbar\partial_j - e\partial_j\alpha)\Psi_2 \tag{5.22}$$

However, the matrix elements of the kinetic momentum $\hat{\Pi}^j = \hat{p}^j - e\hat{A}^j$ are gauge invariant. Indeed we have

$$\begin{aligned}
\hat{\Pi}^j(A)\Psi(x) &\to \hat{\Pi}^j(A')\Psi'(x)\\
&= \left(-i\hbar\partial_j - eA^j + e\partial_j\alpha\right)e^{-\frac{ie}{\hbar}\alpha}\Psi(x)\\
&= e^{-\frac{ie}{\hbar}\alpha}\left(-i\hbar\partial_j - e\partial_j\alpha - eA^j + e\partial_j\alpha\right)\Psi(x)\\
&= e^{-\frac{ie}{\hbar}\alpha}\hat{\Pi}^j(A)\Psi(x) \tag{5.23}
\end{aligned}$$

and so the kinetic momentum $\hat{\Pi}^j(A)$ is a <u>covariant</u> derivative ($\hat{\Pi}^j(A)\Psi$ transforms like Ψ). Thus, when taking matrix elements, the phase factor in eq. (5.23) cancels out and we conclude that the matrix elements of $\hat{\Pi}^j(A)$ are gauge invariant.

Now, what about the gauge covariance of the Hamiltonian and the Schrödinger equation?

Under a gauge transformation the Hamiltonian transforms like:

$$H \xrightarrow{\alpha} H_\alpha = \frac{1}{2m}\left(\hat{p}^i - e\hat{A}^i + e\partial_i\alpha\right)^2 + e\left(\hat{A}_0 + \partial_t\alpha\right) \tag{5.24}$$

Assume now that Ψ solves the Schrödinger equation with respect to H:

$$i\hbar\partial_t\Psi = H\Psi$$

It is a good exercise to check that $\Psi_\alpha = e^{-\frac{ie}{\hbar}\alpha}\Psi$ solves the Schrödinger equation with respect to H_α:

$$i\hbar\partial_t\Psi_\alpha = H_\alpha\Psi_\alpha \tag{5.25}$$

Thus, the Schrödinger equation is gauge covariant.

In the same way, we have that the probability density $\Psi^*\Psi = |\Psi|^2$ is gauge invariant. Then what is the probability current?

It is expectedly given through the velocity operator:

$$\hat{v}^j = \frac{\hat{\Pi}^j}{m} = \frac{1}{m}\left(-i\hbar\partial_j - eA^j\right) \tag{5.26}$$

$$J^j(x) = \frac{1}{2}\left(\Psi^*(x)\hat{v}^j\Psi(x) - \left(\hat{v}^j\Psi(x)\right)^*\Psi(x)\right)$$
$$= \frac{-i}{2m}\left(\Psi^*\left(\hbar\partial_j - ieA^j\right)\Psi - \left(\left(\hbar\partial_j - ieA^j\right)\Psi\right)^*\Psi\right) \tag{5.27}$$

Indeed, by the Schrödinger equation, we can check that $\partial_t|\Psi|^2 + \partial_j J^j = 0$. J^j is also manifestly gauge invariant.

In order to prove current conservation let us define:

$$\overrightarrow{D}_i = \hbar\overrightarrow{\partial}_i - ieA^i$$
$$\overleftarrow{D}_i = \hbar\overleftarrow{\partial}_i + ieA^i \tag{5.28}$$

Using these definitions, we can write:

$$J^j = \frac{-i}{2m}\left(\Psi^*\overrightarrow{D}_j\Psi - \Psi^*\overleftarrow{D}_j\Psi\right)$$
$$\overrightarrow{\partial}_i + \overleftarrow{\partial}_i = \frac{1}{\hbar}\left(\overrightarrow{D}_i + \overleftarrow{D}_i\right)$$
$$\frac{\overrightarrow{D}^2}{2m} = \frac{D^2}{2m} = eA_0 - H \tag{5.29}$$

We can then compute:

$$\partial_j J^j = \frac{-i}{2m\hbar}\left(\Psi^*\left(\overrightarrow{D}_i + \overleftarrow{D}_i\right)\left(\overrightarrow{D}_i\Psi\right) - \left(\Psi^*\overleftarrow{D}_i\right)\left(\overrightarrow{D}_i + \overleftarrow{D}_i\right)\Psi\right)$$
$$= \frac{-i}{2m\hbar}\left(\Psi^*\overrightarrow{D}_i\overrightarrow{D}_i\Psi - \Psi^*\overleftarrow{D}_i\overleftarrow{D}_i\Psi\right)$$
$$= \frac{-i}{2m\hbar}\left(\Psi^*\left(D^2\Psi\right) - \left(D^2\Psi\right)^*\Psi\right)$$
$$= \frac{i}{\hbar}\left(\Psi^*\left(H - eA_0\right)\Psi - \left(\left(H - eA_0\right)\Psi\right)^*\Psi\right)$$
$$= i\left(\Psi^*i\partial_t\Psi - \left(i\partial_t\Psi\right)^*\Psi\right)$$
$$= -\Psi^*\partial_t\Psi - \partial_t\Psi^*\Psi = -\partial_t|\Psi|^2 \tag{5.30}$$

5.2 Particle in a constant magnetic field

Let us now study the system of a particle in a constant magnetic field.

5.2.1 An exercise on translations

Let us first study what happens with spatial translations in this particular case. We take the magnetic field along the z-axis: $\vec{B} = (0, 0, B)$.

We can choose the electromagnetic quadrivector as:

$$\vec{A} = \frac{1}{2}\vec{B} \wedge \vec{r} \quad \Rightarrow \quad A_1 = -\frac{1}{2}By, \ A_2 = \frac{1}{2}Bx \tag{5.31}$$

We then recover the magnetic field by:

$$\vec{B}_3 = \left(\vec{\nabla} \wedge \vec{A}\right)_3 = \epsilon_{321}\partial_2 A_1 + \epsilon_{312}\partial_1 A_2 = -\partial_2 A_1 + \partial_1 A_2 = B \tag{5.32}$$

This possible gauge choice leads to the following Hamiltonian, in the coordinate representation:

$$\hat{H} = \frac{1}{2m}\left(\hat{\Pi}^i(A)\right)^2 = \frac{1}{2m}\left[\left(\hat{p}_1 + \frac{eB}{2}y\right)^2 + \left(\hat{p}_2 - \frac{eB}{2}x\right)^2 + \hat{p}_3{}^2\right] \tag{5.33}$$

How are spatial translations realized?

- $-i\hbar\partial_i$, the naive generators, <u>do not</u> commute with the Hamiltonian.

- Translations along the x and y axis are described by the unitary operator $U(a, b)$ such that $U(a, b)\Psi(x, y) = \Psi(x + a, y + b)$. This operator can be written as $U(a, b) = \exp\left(\frac{ia\hat{p}_1}{\hbar} + \frac{ib\hat{p}_2}{\hbar}\right)$. Its action on operators is $\hat{O}(x + a, y + b) = U(a, b)\hat{O}(x, y)U^\dagger(a, b)$.

Let us now look at the translational invariance of the spectrum of the Hamiltonian. We have:

$$\hat{H}(x, y)\Psi_n(x, y) = E_n\Psi_n(x, y)$$
$$U(a, b)\hat{H}(x, y)\Psi_n(x, y) = E_n U(a, b)\Psi_n(x, y)$$
$$U(a, b)\hat{H}(x, y)U^\dagger(a, b)U(a, b)\Psi_n(x, y) = E_n U(a, b)\Psi_n(x, y)$$
$$\hat{H}(x + a, y + b)\Psi_n(x + a, y + b) = E_n\Psi_n(x + a, y + b) \tag{5.34}$$

However, $\hat{H}(x + a, y + b)$ is related to $\hat{H}(x, y)$ by a gauge transformation:

$$\Rightarrow \begin{cases} \bar{A}_1 = -\frac{1}{2}B(y + b) = -\frac{1}{2}By + \partial_x\left(-\frac{Bbx}{2}\right) \\ \bar{A}_2 = \frac{1}{2}B(x + a) = \frac{1}{2}Bx + \partial_y\left(\frac{Bay}{2}\right) \\ \begin{cases} \bar{A}_\mu = A_\mu + \partial_\mu\alpha \\ \alpha = \frac{B}{2}(ay - bx) \end{cases} \end{cases} \tag{5.35}$$

Thus, we can put these results together and write:

$$e^{\frac{ie}{\hbar}\alpha}\hat{H}(x, y)e^{-\frac{ie}{\hbar}\alpha}\Psi_n(x + a, y + b) = E_n\Psi_n(x + a, y + b) \tag{5.36}$$

We have then the following relation:

$$\begin{cases} \hat{H}(x,y)\tilde{\Psi}_n = E_n\tilde{\Psi}_n \\ \tilde{\Psi}_n = e^{-\frac{ie}{\hbar}\alpha}\Psi_n(x+a, y+b) = e^{i\frac{eB}{2\hbar}(bx-ay)}e^{\frac{i}{\hbar}(a\hat{p}_1+b\hat{p}_2)}\Psi_n(x,y) \end{cases} \quad (5.37)$$

We have thus obtained the infinitesimal generators of translations:

$$T_1 = \hat{p}_1 - \frac{eB}{2}y$$

$$T_2 = \hat{p}_2 + \frac{eB}{2}x \quad (5.38)$$

Notice that these generators commute with Π^1 and Π^2:

$$\left[T_1, \Pi^1\right] = \left[\hat{p}_1 - \frac{eB}{2}y, \hat{p}_1 + \frac{eB}{2}y\right] = 0$$

$$\left[T_1, \Pi^2\right] = \left[\hat{p}_1 - \frac{eB}{2}y, \hat{p}_2 - \frac{eB}{2}x\right] = -\frac{eB}{2}\left([\hat{p}_1, x] + [y, \hat{p}_2]\right) = 0 \quad (5.39)$$

However, T_1 and T_2 do not commute among themselves:

$$[T_1, T_2] = \left[\hat{p}_1 - \frac{eB}{2}y, \hat{p}_2 + \frac{eB}{2}x\right] = \frac{eB}{2}(-i\hbar - i\hbar) = -i\hbar eB \quad (5.40)$$

- The group of translations is thus a projective realization of the classical one.

- The commutator is related to the enclosed flux.

- Previously, we chose one particular way to translate from (x, y) to $(x + a, y + b)$. Any other way would differ by $e^{i\gamma}$, with $\gamma \sim \hbar eB$.

5.2.2 Motion

We want to describe first the classical motion of a particle in this constant magnetic field, oriented along the z-axis: $\vec{B} = (0, 0, B)$. The classical equations of motion give the following result:

- $\ddot{z} = 0 \Rightarrow z = z_0 + v_z t$.

- (x, y) describe circular orbits with frequency $\omega_c = \frac{eB}{m}$. If $eB > 0$, the rotation is clockwise.

  Notice: harmonicity: the frequency is independent of the radius of rotation.

  We get:

$$\begin{cases} x = x_c + R\cos\omega_c t \\ y = y_c - R\sin\omega_c t \end{cases} \quad (5.41)$$

where (x_c, y_c) is the coordinate of the center of rotation. Its time evolution is described by:

$$\begin{cases} x_c = x + \dfrac{1}{\omega_c}\dot{y} = x + \dfrac{1}{\omega_c}\dfrac{\Pi_y}{m} \\ y_c = y - \dfrac{1}{\omega_c}\dot{x} = y - \dfrac{1}{\omega_c}\dfrac{\Pi_x}{m} \end{cases} \quad (5.42)$$

x_c and y_c are two constants of motion. What is the associated symmetry?
The answer is translations in (x, y).

Let us see this directly by working with the quantum Hamiltonian in some
gauge. Remember that we have seen that performing a gauge transformation
on the vector potential amounts to a phase rotation: $\Psi \rightarrow e^{-\frac{ie}{\hbar}\alpha}\Psi$.

Let us pick Landau's gauge which is also convenient to compute energy levels:

$$A_x = -By \qquad A_y = 0 \tag{5.43}$$

The Hamiltonian is:

$$\hat{H} = \frac{1}{2m}\left((\hat{p}_1 + eB\hat{y})^2 + \hat{p}_2{}^2 + \hat{p}_3{}^2\right) \tag{5.44}$$

The kinetic momenta are given by:

$$\begin{cases} \hat{\Pi}_1 = \hat{p}_1 + eB\hat{y} \\ \hat{\Pi}_2 = \hat{p}_2 \\ \hat{\Pi}_3 = \hat{p}_3 \end{cases} \tag{5.45}$$

- Notice that

$$\left[\hat{\Pi}_1, \hat{\Pi}_2\right] = -i\hbar eB \neq 0 \tag{5.46}$$

  The two velocity components in the plane perpendicular to $\vec{B}$ do not
  commute. Thus, they cannot be measured simultaneously with arbitrary
  accuracy.

- The combinations

$$\begin{cases} T_1 = \hat{p}_1 \\ T_2 = \hat{p}_2 + eBx \end{cases} \tag{5.47}$$

  commute with $\hat{\Pi}_{1,2,3}$. Thus, $[T_i, H] = 0$, which implies that they are
  conserved.

  They indeed correspond to the coordinates of the center of the classical
  motion. Comparing them to (5.42), we get:

$$\begin{cases} T_1 = \Pi_1 - eBy = -eBy_c \\ T_2 = \Pi_2 + eBx = eBx_c \end{cases} \tag{5.48}$$

- Quantum mechanically, also T_1 and T_2 cannot be fixed simultaneously as

$$[T_1, T_2] = -i\hbar eB \tag{5.49}$$

- Given a solution of the Schrödinger equation $\Psi(x, y, z)$, then

$$\Psi_{a,b}(x, y, z) = e^{\frac{i}{\hbar}(aT_1 + bT_2)}\Psi(x, y, z) \tag{5.50}$$

  is also a solution. What does this operation represent?
  It is a space translation.

This fact is obvious for $e^{i\frac{aT_1}{\hbar}} = e^{i\frac{a\hat{p}_1}{\hbar}} = e^{a\partial_x}$.

For $e^{i\frac{bT_2}{\hbar}}$, we have:

$$e^{i\frac{bT_2}{\hbar}}\Psi(x,y,z) = e^{i\frac{eBx}{\hbar}}e^{b\partial_y}\Psi(x,y,z) = e^{i\frac{eBx}{\hbar}}\Psi(x,y+b,z)$$

This is an ordinary translation composed with a gauge transformation.

- Notice that $[T_1, T_2] \neq 0$ implies that the translation group is non-commutative in presence of a magnetic field.

To be stressed and to conclude:

The pairs of canonically conjugated variables are $(\hat{\Pi}_1, \hat{\Pi}_2)$, which are physical velocities, and (T_1, T_2) which are the coordinates of the center of the orbit.

In a magnetic field, the canonically conjugated variables are (velocity,velocity) and (position,position), whereas in ordinary motion in a potential those are (velocity,position).

5.2.3 Landau levels

In order to study the Landau quantization, let us continue working in the Landau gauge:

$$A_x = -By \qquad A_y = 0 \tag{5.51}$$

- The rotation invariance around $(x, y) = 0$ is not manifest.

- The translational invariance in the x-direction is manifestly preserved, whereas it is not manifest in the y-direction.

We have the Hamiltonian:

$$\hat{H} = \frac{1}{2m}\left((\hat{p}_1 + eB\hat{y})^2 + \hat{p}_2{}^2 + \hat{p}_3{}^2\right) \tag{5.52}$$

As $\hat{p}_1$ and $\hat{p}_3$ commute with $\hat{H}$, we can choose (p_3, p_1, E) as quantum numbers:

$$\hat{p}_3\Psi = p_3\Psi$$
$$\hat{p}_1\Psi = p_1\Psi$$
$$\hat{H}\Psi = E\Psi \tag{5.53}$$

Such a state will satisfy:

$$\Psi(x,y,z) = e^{\frac{i}{\hbar}(p_1 x + p_3 z)}F(y) \tag{5.54}$$

For such a state, the Hamiltonian is equivalent to:

$$\hat{H} = \frac{1}{2m}\left((p_1 + eB\hat{y})^2 + \hat{p}_2{}^2 + p_3{}^2\right) \tag{5.55}$$

It is the Hamiltonian of a harmonic oscillator in $(\hat{p}_2, \hat{y})$ with frequency $\omega_c = \frac{eB}{m}$, which is the cyclotron frequency of the particle, and centered at $y_c = -\frac{p_1}{eB} = -\frac{p_1}{m\omega_c}$:

$$\hat{H} = \frac{1}{2m}\hat{p}_2{}^2 + \frac{1}{2}m\left(\frac{eB}{m}\right)^2\left(\hat{y} + \frac{p_1}{eB}\right)^2 + \frac{p_3{}^2}{2m} \tag{5.56}$$

By quantizing this harmonic oscillator in $(\hat{p}_2, \hat{y})$, we get the energy levels:

$$E(p_3, p_1, n) = \frac{p_3{}^2}{2m} + \hbar\omega_c \left(n + \frac{1}{2}\right) \tag{5.57}$$

with the wave functions:

$$\Psi_{p_3, p_1, n}(x, y, z) = e^{-\frac{i}{\hbar}(p_1 x + p_3 z)} \Psi_n \left(y + \frac{p_1}{m\omega_c}\right)$$

$$\Psi_n(y) = \left(\frac{m\omega_c}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n \left(y\sqrt{\frac{m\omega_c}{\hbar}}\right) e^{-\frac{m\omega_c{}^2 y^2}{2\hbar}} \tag{5.58}$$

where $\Psi_n(y)$ is the ordinary wave function of a harmonic oscillator around $y = 0$ with frequency ω_c, and $H_n(x)$ are the Hermite polynomials defined as:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \tag{5.59}$$

- The energy is degenerate in $p_1 \sim y_c$. This is related to translational invariance.

- The result (5.57) is in accord with the classical property of the system: the frequency of rotation does not depend on the radius: this is harmonicity.

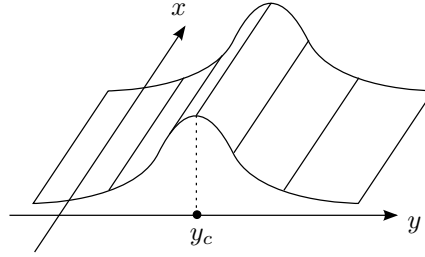- The shape of $|\Psi_{p_3, p_1, n=0}(x, y)|$ is depicted in figure 5.1.

Figure 5.1: The shape of the norm of the wavefunction $\Psi_{p_3, p_1, n=0}(x, y)$. We see that it is far from rotational invariant.

Where is cylindrical symmetry gone? To make it manifest, we must superimpose different wavefunctions:

$$\Psi_{p_3, n_2, n}(x, y, z) = \int dp_1 \Psi_{p_3, p_1, n}(x, y, z) f(p_1, n_2) \tag{5.60}$$

- In Landau gauge, we have:

$$\hat{\Pi}_2 = \hat{p}_2 \qquad\qquad \hat{\Pi}_1 = \hat{p}_1 + eB\hat{y}$$
$$T_1 = \hat{p}_1 \qquad\qquad T_2 = \hat{p}_2 + eB\hat{x} \tag{5.61}$$

We can check that:

$$\left[\hat{\Pi}_1, T_2\right] = eB \left([\hat{p}_1, \hat{x}] + [\hat{y}, \hat{p}_2]\right) = 0 \tag{5.62}$$

We get:

$$m\omega_c \hat{y} = \hat{\Pi}_1 - T_1$$
$$m\omega_c \hat{x} = T_2 - \hat{\Pi}_2 \tag{5.63}$$

We can thus conclude that in Landau gauge, for the states $\Psi_{p_3,p_1,n}$, $y_c = -\frac{T_1}{m\omega_c}$ is fixed, whereas $x_c = \frac{T_2}{m\omega_c}$ is not, and is fully spread.

It is intructive to count the levels for the case where the motion is limited to a region of sides L_x, L_y in the plane.

If the motion is limited to $0 \leqslant x \leqslant L_x$, then p_1 is quantized:

$$p_1 = \frac{2\pi\hbar}{L_x} n_2 \qquad n_2 \in \mathbb{Z} \tag{5.64}$$

Thus, the position y_c is quantized:

$$y_c = \frac{p_1}{eB} = \frac{2\pi\hbar}{eBL_x} n_2 \tag{5.65}$$

Note that it is the case whether or not the motion is limited in the y direction!

Now, if the motion is limited in the y direction as $0 \leqslant y \leqslant L_y$, then the number of states of quantum numbers (n, p_3) we can fit in is:

$$N(n, p_3) = \frac{L_y}{\Delta y_c} = \frac{L_x L_y}{2\pi\hbar} eB \tag{5.66}$$

5.3 The Aharonov-Bohm effect

The study of the vector potential in quantum mechanics opens a window on deeper aspects of the quantum world, some of which have a full description only in quantum field theory:

1. The relevance of topology

2. The charge quantization

The Aharonov-Bohm effect is one remarkable and yet simple example.

Consider an ideal infinitely long and empty cylindrical shell such that particles do not have access to its interior. The propagation of particles in this setup is characterized by a Schrödinger equation with boundary condition $\Psi(x, y, z) = 0$ on the surface of the cylinder. In the path integral approach, this corresponds to summing only on paths that do not go through the interior of the cylinder.

Imagine now a modified arrangement where the cylindrical shell encloses a uniform magnetic field (see figure 5.2). This could, for instance, be realized by placing an "infinitely" long solenoid inside the shell.

Intuitively, we would think that physics (the propagation of charged particles) is unaffected outside the shell, as $\vec{B} = 0$ there. However, quantum mechanics tells that this conjecture is wrong!

To show this, we must consider the vector potential. Outside the shell, $\vec{B} = 0$, but $\vec{A} \neq 0$ as implied by Stokes' theorem (see figure 5.3).
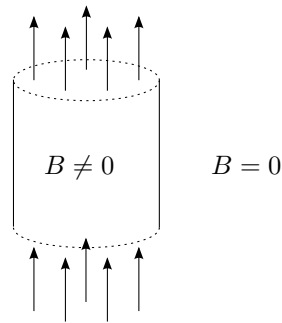
Figure 5.2: An infinitely long cylinder has a constant magnetic field inside it, whereas outside it there is no magnetic field.

$$\gamma = \partial\sigma$$

$$\oint_{\gamma} \vec{A} \cdot d\vec{x} = \int_{\sigma} \vec{B} \cdot d\vec{\sigma} = BS$$
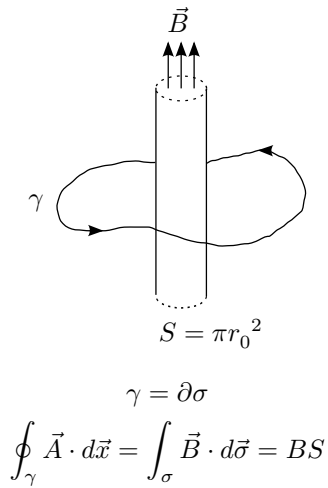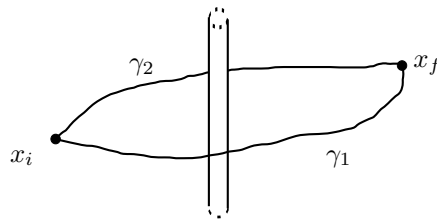
Figure 5.3: An infinitely long cylinder has a constant magnetic field inside it, whereas outside it there is no magnetic field.

Figure 5.4: Two paths γ_1 and γ_2 from x_i to x_f that cannot be continuously deformed into each other, due to the topological defect between them.

One possible gauge choice (the only one that manifestly respects cylindrical symmetry) is $A_\phi = \frac{BS}{2\pi r}$, $A_r, A_z = 0$ in cylindrical coordinates, for $r > r_0$.

It is immediate to see that A_ϕ has physical consequences by considering quantum amplitudes in the path integral approach. Consider two paths γ_1 and γ_2 like in figure 5.4.

- γ_1 cannot be continuously deformed into γ_2.

- They are topologically inequivalent (they belong to different homotopy classes).

Consider the contribution of γ_1 and γ_2 to $K(x_f, x_i; t)$:

$$\gamma_1 \to e^{\frac{iS_1}{\hbar}} = \exp\left(\frac{iS_0^{(1)}}{\hbar} - \frac{ie}{\hbar}\int_{\gamma_1} A^i dx^i\right)$$

$$\gamma_2 \to e^{\frac{iS_2}{\hbar}} = \exp\left(\frac{iS_0^{(2)}}{\hbar} - \frac{ie}{\hbar}\int_{\gamma_2} A^i dx^i\right) \tag{5.67}$$

where $S_0^{(i)}$ is the free particle action for γ_i.

The phase difference induced by the vector potential is:

$$\Delta\phi = \frac{e}{\hbar}\left(\int_{\gamma_2} A^i dx^i - \int_{\gamma_1} A^i dx^i\right) = \frac{e}{\hbar}\oint_{\gamma_2 - \gamma_1} A^i dx^i = -\frac{eBS}{\hbar} \equiv -\frac{e\Phi}{\hbar} \tag{5.68}$$

1. Apparently the presence of the solenoid is felt at the quantum level by trajectories that are arbitrarily far from it!

2. Notice that the phase shift vanishes between paths that are topologically equivalent, since they do not encircle any magnetic flux.

The suprising relevance of the vector potential at the quantum level was first suggested by Aharonov and Bohm (1959) and later tested by Chambers (1960) and more recently by Tonomura (1982).

The ideal "obvious" way to test this effect is to perform the double slit experiment in the presence of our infinite and thin solenoid (in reality the solenoid is replaced by a thin magnetized iron filament called a whisker), as in figure 5.5.

Two disjoint classes of trajectories contribute to the propagation amplitude from the source S to the screen C:

$$K(x_f, x_i; t) = \int \mathscr{D}[x]_{\gamma_1} e^{\frac{i}{\hbar}\left(S_0^{(1)} - e\int A^i dx^i\right)} + \int \mathscr{D}[x]_{\gamma_2} e^{\frac{i}{\hbar}\left(S_0^{(2)} - e\int A^i dx^i\right)} \tag{5.69}$$

By Stokes' theorem, $\int_{\gamma_1} A^i dx^i$ is the same for all trajectories in the class 1 (i.e. passing on the top of the solenoid). The same thing is true for the class 2.

Moreover, we have:

$$\int_{\gamma_1} A^i dx^i - \int_{\gamma_2} A^i dx^i = \oint_{\gamma_1 - \gamma_2} A^i dx^i = BS = \Phi \tag{5.70}$$

where Φ is the magnetic flux through the solenoid.

Thus, the total contribution will be:

$$K(x_f, x_i; t) = e^{-\frac{ie}{\hbar}\int_{\gamma_1} A^i dx^i}\left(\phi_1^{(0)}(x_f) + e^{\frac{ie}{\hbar}\Phi}\phi_2^{(0)}(x_f)\right)$$

$$= e^{i\alpha}\left(\phi_1^{(0)}(x_f) + e^{\frac{ie}{\hbar}\Phi}\phi_2^{(0)}(x_f)\right) \tag{5.71}$$
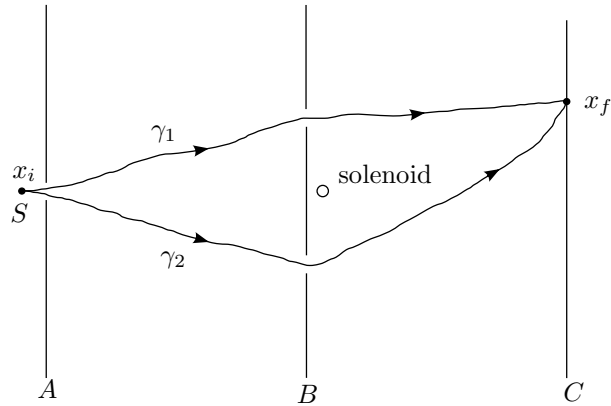
Figure 5.5: The experimental setup to test the Aharonov-Bohm effect. The two paths γ_1 and γ_2 contribute to the propagation amplitude from the source S to the screen C differently.

where $\phi_i^{(0)}$ is the contribution of the class i in the absence of the solenoid.

The final amplitude will be:

$$|K|^2 = \left|\phi_1^{(0)}\right|^2 + \left|\phi_2^{(0)}\right|^2 + 2\operatorname{Re}\left(\phi_1^{(0)*} e^{\frac{ie}{\hbar}\Phi}\phi_2^{(0)}\right) = F_1 + F_2 + F_{int} \qquad (5.72)$$

This result tells us what the effect of the solenoid is, no matter how complicated $\phi_i^{(0)}$ are. This is because its effect is purely topological: the only property of the trajectory that enters into the phase shift is its topology (whether it belongs to the class 1 or 2).

In the case of the free propagation, we have (see figure 5.6):

$$\phi_1^{(0)*}\phi_2^{(0)} = e^{2\frac{i}{\hbar}\frac{ka}{b}z} \equiv e^{2\frac{i}{\hbar}k_{\parallel}z}$$

$$\Rightarrow\ F_{int} = 2\operatorname{Re}\left(e^{i\left(\frac{2k_{\parallel}z}{\hbar}+\frac{e\Phi}{\hbar}\right)}\right) = 2\cos\left(\frac{2k_{\parallel}z}{\hbar}+\frac{e\Phi}{\hbar}\right) \qquad (5.73)$$

Thus, as Φ is varied, the peaks of the interference pattern are shifted along the z direction.

This effect is periodic in the flux Φ with period:

$$\Phi_0 \equiv \Delta\Phi = \frac{2\pi\hbar}{e} = 4.135 \cdot 10^{-7} \text{ gauss} \times \text{cm}^2 \qquad (5.74)$$

which represents a fundamental unit of magnetic flux.

The effect of the solenoid vanishes for $\Phi = n\Phi_0$.

Moral:

1. The Aharonov-Bohm effect shows that $F_{\mu\nu}$ underdescribes electromagnetism; i.e. different physical situations in a region may have the same $F_{\mu\nu}$ in that region.
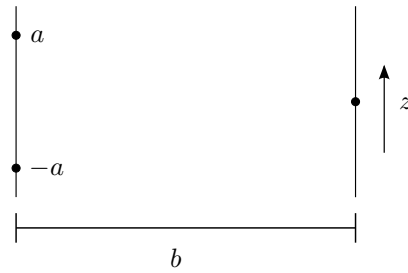
Figure 5.6: The experimental setup to test the Aharonov-Bohm effect. The two slits are located at a and $-a$ along the vertical direction, the two screens are separated by a distance b, and the position on the final screen is described by z.

2. The phase $\varphi = \frac{e}{\hbar} \oint A^i dx^i$ <u>overdescribes</u> electromagnetism; i.e. different phases in a region may describe the same physics. For example $\Phi' = \Phi + n\Phi_0$.

3. What provides a complete description is the factor $e^{i\varphi} = e^{\frac{ie}{\hbar} \oint_\gamma A_\mu dx^\mu}$ over all possible closed paths in space-time, which after all is what enters in the path integral.

Thus, electromagnetism is the gauge invariant manifestation of a non-integrable phase factor, as stated by Yang and Wu (1975).

5.3.1 Energy levels

Let us now do a simple example on the energy levels of a charged particle confined on a ring of radius R around a solenoid (see figure 5.7).
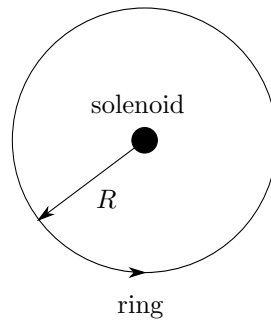

Figure 5.7: A particle is confined on a ring of radius R around a solenoid of area σ went through by a magnetic field of intensity B.

The vector potential describing this situation is such that:

$$\int_\sigma B d\sigma = \oint_{\partial\sigma} \vec{A} d\vec{x} \tag{5.75}$$

The magnetic flux is found to be:

$$\Phi = B\sigma = A_\theta(R)2\pi R \tag{5.76}$$

Which fixes the phase factor:

$$e^{-\frac{ie}{\hbar}\oint \vec{A}d\vec{x}} = e^{-i\frac{e\Phi}{\hbar}} \equiv e^{-i\varphi} \tag{5.77}$$

We then find the Hamiltonian for the particle:

$$H = \frac{1}{2m}\left(p_\theta - eA_\theta\right)^2 = \frac{1}{2m}\left(-\frac{i\hbar\partial_\theta}{R} - \frac{e\Phi}{2\pi R}\right)^2$$

$$= \frac{1}{2m}\frac{\hbar^2}{R^2}\left(-i\partial_\theta - \frac{e\Phi}{2\pi\hbar}\right)^2 = \frac{1}{2m}\frac{\hbar^2}{R^2}\left(-i\partial_\theta - \frac{\varphi}{2\pi}\right)^2 \tag{5.78}$$

The eigenstates of this Hamiltonian are:

$$\Psi_n(\theta) = e^{in\theta} \qquad n \in \mathbb{Z} \tag{5.79}$$

with energy levels:

$$E_n = \frac{1}{2m}\frac{\hbar^2}{R^2}\left(n - \frac{\varphi}{2\pi}\right)^2 = \frac{1}{2m}\frac{\hbar^2}{R^2}\left(n - \alpha\right)^2 \tag{5.80}$$

We can notice that when $\varphi \to \varphi + 2\pi m$, with m an integer, $\alpha \to \alpha + m$, and thus the spectrum is the same.

The conclusion is that what is physical is not φ itself, but the phase factor $e^{i\varphi}$. Moreover, the physical angular momentum $Rp_\theta = \hbar(n-\alpha)$ is not quantized in integer units of $\hbar$.

5.4 Dirac's magnetic monopole

Let us now very briefly and qualitatively discuss Dirac's magnetic monopole.

Let us take our thin solenoid and cut it in two: the flux will "expand" out.

The tip of the solenoid will act more or less as a point source of magnetic field: a magnetic monopole (see figure 5.8).

Of course $\vec{\nabla}\cdot\vec{B} = 0$ is still satisfied: the magnetic flux is conserved as there is the "incoming" flux from the solenoid.

Notice that:

$$g_M \equiv \int_\sigma \vec{B}\cdot d\vec{\sigma} \quad \Rightarrow \quad B \approx \frac{g_M}{4\pi r^2} \tag{5.81}$$

where σ is a sphere centered at the end of the solenoid, with the surface where the solenoid crosses it excluded.

Assume now the ideal limit in which the solenoid is infinitely thin.

If for all charged particles the charge e_j the flux Φ satisfies:

$$\frac{e_j\Phi}{\hbar} = 2\pi n_j \tag{5.82}$$

there will be no way to tell the presence of the solenoid (also called Dirac's string). Our object will behave by all means as a point-like magnetic monopole!
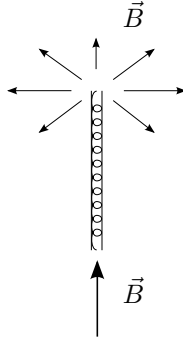
Let us now turn the argument around:

Figure 5.8: The solenoid cut in two will act as a magnetic monopole. Maxwell's second law is still satisfied as the magnetic flux is incoming from the solenoid.

Postulate: magnetic monopoles <u>must</u> exist in order to <u>restore</u> the symmetry between magnetic charge and electric charge which is apparently broken by Maxwell's equations:

$$\vec{\nabla} \cdot \vec{E} = \rho_E \qquad \vec{\nabla} \cdot \vec{B} = 0 \tag{5.83}$$

Since $\vec{\nabla} \cdot \vec{B} = 0$ follows not from dynamics but from kinematics: $B_i = \epsilon_{ijk}\partial_j A_k$, a monopole state must involve an incoming flux localized into some string; but in order to preserve spherical symmetry the string should be <u>undetectable</u>. Thus, the Aharonov-Bohm phase should be a multiple of 2π for all existing electrically charged particles:

$$\frac{e_j g_M}{\hbar} = 2\pi n_j \tag{5.84}$$

Thus, the existence of a single monopole in the universe implies the quantization of the electric charge!

5.4.1 On coupling constants, and why monopoles are different than ordinary charged particles

The strength of the electromagnetic interactions is set by the fine structure constant:

$$\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137} \ll 1 \tag{5.85}$$

The electromagnetic interactions are thus "weak".

The quantization condition implies that the minimal magnetic charge of a monopole, if it existed, is:

$$g_{min} = \frac{2\pi\hbar}{e} \tag{5.86}$$

Thus, the <u>magnetic coupling constant</u>, α_M, is defined as:

$$\alpha_M = \frac{g_{min}{}^2 c}{\hbar} = \frac{(2\pi)^2 \hbar c}{e^2} = \frac{(2\pi)^2}{\alpha} \approx 137 \cdot (2\pi)^2 \gg 1 \tag{5.87}$$

The magnetic interactions among monopoles are therefore very strong!

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[2] "Path Integral Methods and Applications", R. MacKenzie, arXiv:quant-ph/0004090. (readable overview on the subject)

The following books may be of help in complementing the lecture notes.

[3] "Modern Quantum Mechanics", J.J. Sakurai, The Benjamin/Cummings Publishing Company, 1985. (chapters 2.5 and 2.6: quick introduction to path integral and nice extended discussion of electromagnetic interactions, Aharonov-Bohm, monopoles)

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[5] "Path Integrals in Quantum Mechanics, Statistics and Polymer Physics", Hagen Kleinert, World Scientific, 1995. Chapter 3, in particular sections 3.9, 3.10 and 3.11 give a good account of Feynman diagrams

[6] "Topics in Advanced Quantum mechanics", Barry R. Holstein, Addison-Wesley 1982. Chapters 1 and 5 (contains a lot of subjects, which is nice, but sometimes he is too sloppy)

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