Quantum Physics IV
EPFL

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July 3, 2024

Abstract

This a summary of the physics master course "Quantum Physics IV".

Contents

Introduction

This course is an introduction to the path integral formalism of Quantum Mechanics. Familiarity with the standard formulation of Quantum Mechanics is assumed. The course requires some mathematical background. In appendix A, we summarize some of the relevant concepts.

These notes are heavily based on similar lecture notes by Riccardo Rattazzi from 2011. The following books are useful complementary reading for this course:

- "Quantum Mechanics and Path Integrals" , R.P. Feynman and A.R. Hibbs, McGraw-Hill, 1965.
- "Techniques and applications of Path Integration", L.S. Schulman, John Wiley & Sons Inc., 1981.
- "Path Integral Methods and Applications", R. MacKenzie, arXiv:quant-ph/0004090.
- "Modern Quantum Mechanics", J.J. Sakurai, The Benjamin/Cummings Publishing Company, 1985.
- "Aspects of Symmetry", S. Coleman, Cambridge University Press, 1985.
- "Path Integrals in Quantum Mechanics, Statistics and Polymer Physics", Hagen Kleinert, World Scientific, 1995.

Chapter 1

The path integral formalism

Lecture 1 - From the double slit experiment to path integrals

Axioms of (practical) Quantum Mechanics

1. The state of an isolated system is a vector $|\psi\rangle$ in a **Hilbert space** $\mathcal{H}$. State vectors are normalized: $\langle\psi|\psi\rangle = 1$.

2. The state evolves in time according to the Schrödinger equation

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

   where $\hat{H}$ is a hermitian operator called the **Hamiltonian**.

3. An observable O is associated to a hermitian operator $\hat{O}$. The expectation value of O on the state $|\psi\rangle$ is given by $\langle\psi|\hat{O}|\psi\rangle$. This can be used to determine the probability of obtaining a specific value. Writing $\hat{O} = \sum_\lambda \lambda \hat{P}_\lambda$, where $\hat{P}_\lambda$ is the projector onto the subspace of $\mathcal{H}$ associated to the eigenvalue λ of $\hat{O}$, we conclude that the probability of measuring $O = \lambda$ is $\langle\psi|\hat{P}_\lambda|\psi\rangle$ (**Born rule**).

4. After the measurement of an observable O, the state $|\psi\rangle$ **collapses** into the state $\hat{P}_\lambda|\psi\rangle / \sqrt{\langle\psi|\hat{P}_\lambda|\psi\rangle}$, where λ is the value obtained in the measurement.

This is the usual formulation of quantum mechanics often called the Copenhagen interpretation. Clearly, there is tension between axioms 2 and 4 because they give two different rules for time evolution. In addition, one may ask *what is a measurement?* We shall see that axiom 4 is not necessary once we include the "measurement" in the Hamiltonian of the full system. Nevertheless, the debate continues between different interpretations of Quantum Mechanics.

Path integral formulation

The path integral formulation of quantum mechanics is **equivalent** to the usual one described above. Schematically, it states that the probability that a particle travels from

x_i at time t_i to x_f at time t_f is given by

$$\text{Probability}(x_i, t_i \to x_f, t_f) = \left| \sum_{\substack{\text{paths } x(t) \\ x(t_i)=x_i \\ x(t_f)=x_f}} \exp\left(\frac{i}{\hbar} S[x(t)]\right) \right|^2 ,$$

where $S[x(t)]$ is the classical action of the path $x(t)$. The path integral formulation has several **advantages**:

- The classical limit is straightforward.
- There is a clear interpretation of interference (double-slit experiment).
- The path integral in quantum field theory is manifestly Lorentz invariant.
- Non-perturbative phenomena such as instantons are described more easily.
- There is a clear connection with statistical mechanics and the related numerical methods (e.g. Path Integral Monte Carlo).

The double-slit experiment

Before deriving a rigorous formula for the path integral from the Schrödinger picture, we motivate it by considering the double slit experiment. The setup is the following: a screen measures the flux of electrons coming from the source. These electrons are blocked by a wall with two slits, denoted 1 and 2 in figure (1.1). The two slits can be opened or closed.

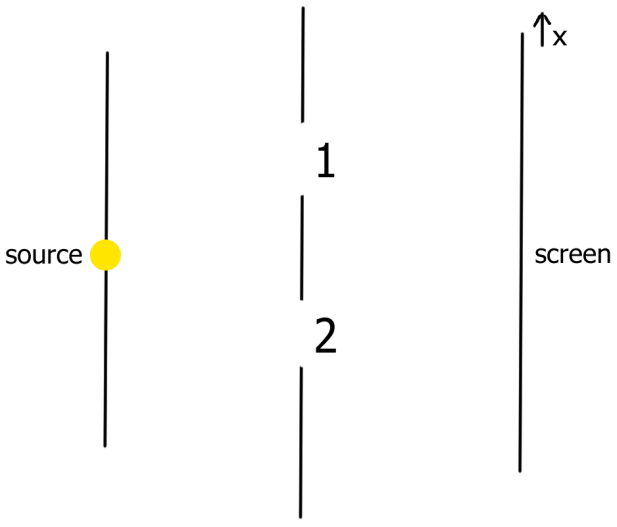
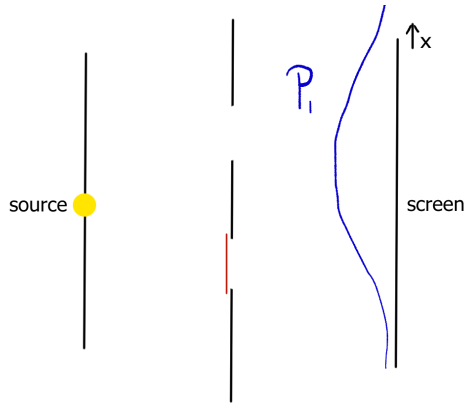
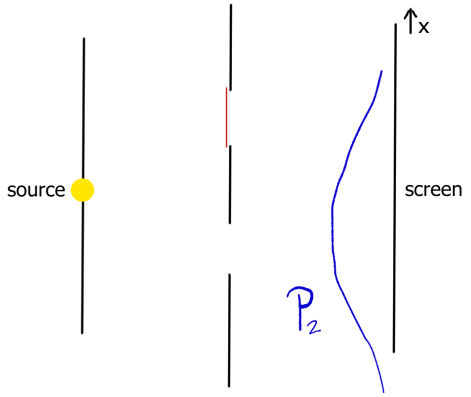


Figure 1.1: The double slit experiment: an electron source and a screen are separated by a wall with two slits, so that the electrons have to pass through slit 1 or slit 2. We measure the electron flux on the screen.

When slit 1 is open and slit 2 is closed, we measure a flux P_1 on the screen (fig 1.2a). Similarly, when slit 2 is open and slit 1 is closed, we measure a flux P_2 on the screen (fig 1.2b)



(a) Slit 1 is open, slit 2 is closed. P_1 is the distribution of electrons on the screen



(b) Slit 2 is open, slit 1 is closed. P_2 is the distribution of electrons on the screen

Figure 1.2: The double slit experiment in the configurations where one slit is closed and the other is open.

However, if both slits are open, the electron distribution on the screen, P, is **not** equal to the sum $P_1 + P_2$ (fig 1.3)[1]. There is an interference pattern, as if the electrons behaved like waves.

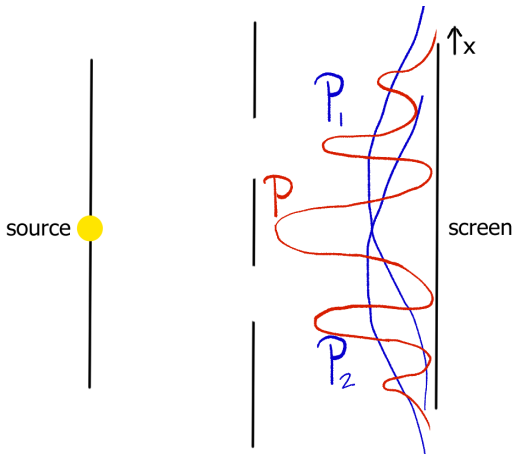


Figure 1.3: The double slit experiment when both slits are open. $P \neq P_1 + P_2$ is the electron distribution on the screen, exhibiting a clear interference pattern.

[1]This figure is not meant to depict the precise interference pattern. A real paper describing the experiment can be found in [1]. The interference pattern itself can be found at `https://commons.wikimedia.org/wiki/File:Single_slit_and_double_slit2.jpg`.

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

The reason for the interference is then straightforward: the distributions P_1 and P_2 are the modulus squared of amplitudes φ_1 and φ_2. P is then obtained by summing the amplitudes, and **then** computing the modulus squared:

$$\left.\begin{aligned} P_1 &= |\varphi_1|^2 \\ P_2 &= |\varphi_2|^2 \end{aligned}\right\} \implies P = \left|\frac{\varphi_1 + \varphi_2}{\sqrt{2}}\right|^2 = \frac{1}{2}(P_1 + P_2 + P_{\text{int}})$$

"In quantum mechanics, you sum amplitudes, not probabilities."

We can complicate the setup further by placing two detectors around each slit. The detectors flash when an electron passes through the corresponding slit (1.4). However, the detectors are not 100% accurate: sometimes the electron arrives at the screen without any detector flashing.

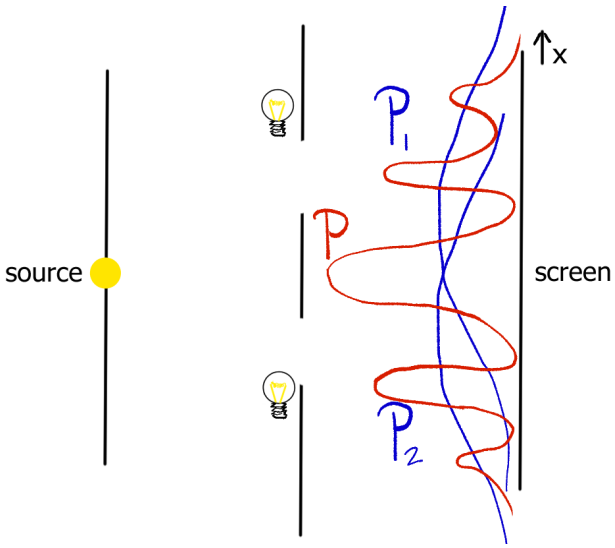


Figure 1.4: The double slit experiment with detectors on each slit. The light bulb flashes when an electron goes through the corresponding slit, but it is not 100% accurate: sometimes there is no flash.

Then, the position on the screen of each individual electron is recorded and labelled $x_1, x_2, \ldots$. Furthermore, we add a superscript that denotes whether the slit 1 flashed ($x^{(1)}$), the slit 2 flashed ($x^{(2)}$), or if there was no flash ($x^{(0)}$). After sending a large number of electrons, we organize the data as in (table 1.1).

	Slit 1	Slit 2	No flash
Coordinates on screen	$x_1^{(1)}$ $x_6^{(1)}$ $\vdots$	$x_2^{(2)}$ $x_3^{(2)}$ $\vdots$	$x_4^{(0)}$ $x_5^{(0)}$ $\vdots$
Electron distribution	P_1	P_2	P

Table 1.1: Example of a possible set of measurements in the double slit experiment with detectors.

The distributions for the data points in each column correspond to P_1, P_2 and P respectively. If we detect an electron in one slit, it is the same as if we block the other slit.

According to the Copenhagen interpretation, the detectors influence the behavior of the electrons: their state collapses after being measured in either slit 1 or 2, therefore destroying the interference pattern. If the detectors miss an electron, as is the case when there is no flash, then the state does not collapse and interference happens.

This is a good opportunity to explain why the collapse of the wave-function is not necessary. In the double-slit experiment without detectors, the time evolution of the particle's wave function is as follows

$$|x=0\rangle \to \frac{1}{\sqrt{2}}\left(|x_{up}\rangle + |x_{down}\rangle\right) \to \int dx \frac{1}{\sqrt{2}}\left(\varphi_1(x)\,|x\rangle + \varphi_2(x)\,|x\rangle\right) \tag{1.1}$$

where the intermediate step corresponds to passing through the (up and down) slits. Therefore, the probability of finding the particle at position $x \in [a,b]$ is given by

$$\langle\psi|\,\mathbb{P}_{[a,b]}\,|\psi\rangle = \int_a^b dx \frac{1}{2}|\varphi_1(x) + \varphi_2(x)|^2 \tag{1.2}$$

Let us now model each detector by a qubit that takes value 0 if no electron was detected and 1 otherwise. For simplicity, let us assume that the detectors are infallible. Then the time evolution of the state of the system is given by:

$$\begin{aligned} |x=0, q_1=0, q_2=0\rangle &\to \frac{1}{\sqrt{2}}\left(|x_{up}, q_1=1, q_2=0\rangle + |x_{down}, q_1=0, q_2=1\rangle\right) \\ &\to \int dx \frac{1}{\sqrt{2}}\left(\varphi_1(x)\,|x, q_1=1, q_2=0\rangle + \varphi_2(x)\,|x, q_1=0, q_2=1\rangle\right) \end{aligned} \tag{1.3}$$

where we denoted the detector qubits by q_1 and q_2. In this case, the probability of finding the particle at position $x \in [a,b]$ is given by

$$\langle\psi|\,\mathbb{P}_{[a,b]}\,|\psi\rangle = \int_a^b dx \frac{1}{2}\left(|\varphi_1(x)|^2 + |\varphi_2(x)|^2\right) \tag{1.4}$$

because of the orthogonality $\langle x, q_1=1, q_2=0|x', q_1=0, q_2=1\rangle = 0$. Therefore, if there is any degree of freedom that changes its state depending on which slit the electron

passes then the interference pattern will be lost. This is the reason why it is so difficult to perform double slit experiments with larger objects [2]. This is also the reason why quantum communication can be very safe.

Now in order to motivate the path integral formulation, imagine a N-slit experiment with M walls (figure 1.5)

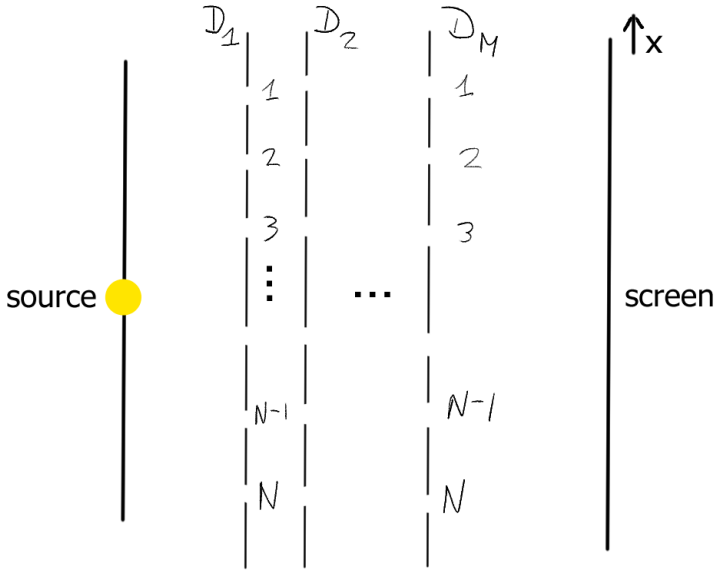


Figure 1.5: N-slit experiment with M walls.

Now the probability distribution on the screen will be given, as before, by some amplitude squared $|\varphi|^2$. There are now several different amplitudes associated to the different paths that the electron might take to go through the slits. For example, $\varphi(x_{D_1,1}, x_{D_2,2}, x_{D_3,1}, \ldots)$ is the amplitude for a trajectory passing through slit 1 in the first wall, slit 2 in the second wall, and slit 1 in the third wall.

By superposition, the amplitude on the final screen is given by summing the amplitudes corresponding to the different paths:

$$\varphi = \sum_{j_1=1}^{N} \sum_{j_2=1}^{N} \cdots \sum_{j_M=1}^{N} \varphi(x_{D_1,j_1}, x_{D_2,j_2}, \ldots, x_{D_M,j_M}).$$

As we consider more and more slits in each wall, we approach the situation where there is no wall at all. Mathematically, this corresponds to taking the limit $N \to \infty$, and the sums become integrals:

$$\varphi = \int \mathrm{d}x_1 \ldots \mathrm{d}x_M \, \varphi(x_1, \ldots, x_M). \tag{1.5}$$

Intuitively, we have an amplitude for each possible trajectory of the electron, and we then integrate over all possible trajectories.

From the Schrödinger approach to the path integral

We begin by defining the **propagator**

$$K(x_f,t_f;x_i,t_i) \equiv \langle x_f|\, e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}\,|x_i\rangle\,, \quad \hat{H}=\frac{\hat{p}^2}{2m}+V(\hat{x}). \tag{1.6}$$

We then divide the time interval into N steps of size ϵ:

$$t=t_f-t_i=N\epsilon, \quad 0<\epsilon\ll 1.$$

We will then take the limit $N\to\infty$ (or $\epsilon\to 0$) at the end of the computation. Using this, we can write

$$K(x_f,t_f;x_i,t_i)=\langle x_f|\underbrace{e^{-\frac{i}{\hbar}\hat{H}\epsilon}\dots e^{-\frac{i}{\hbar}\hat{H}\epsilon}}_{N\text{ times}}|x_i\rangle \tag{1.7}$$

Now between each exponential we insert a completeness relation ($1=\int \mathrm{d}x\,|x\rangle\langle x|$). Overall, $N-1$ completeness relations are inserted, and there are therefore $N-1$ integration variables $x_1,x_2,\dots x_{N-1}$. For ease of notation, we set $x_N\equiv x_f$ and $x_0\equiv x_i$.

$$\begin{aligned}K(x_f,t_f;x_i,t_i)&=\langle x_N|\, e^{-\frac{i}{\hbar}\hat{H}\epsilon}\int \mathrm{d}x_{N-1}\,|x_{N-1}\rangle\langle x_{N-1}|\dots\int \mathrm{d}x_1\,|x_1\rangle\langle x_1|\, e^{-\frac{i}{\hbar}\hat{H}\epsilon}\,|x_0\rangle\\&=\int \mathrm{d}x_{N-1}\dots\mathrm{d}x_1\prod_{k=1}^{N}\langle x_k|\, e^{-\frac{i}{\hbar}\hat{H}\epsilon}\,|x_{k-1}\rangle\end{aligned} \tag{1.8}$$

Consider then[2]

$$\left\langle x'\right|\, e^{-\frac{i}{\hbar}\hat{H}\epsilon}\,|x\rangle=\int \mathrm{d}p\,\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px'}\,\langle p|\, e^{-\frac{i}{\hbar}\hat{H}\epsilon}\,|x\rangle\,. \tag{1.9}$$

The Zassenhaus formula (A.3) allows to compute the matrix element $\langle p|\, e^{-\frac{i}{\hbar}\hat{H}\epsilon}\,|x\rangle$ in the limit $\epsilon\to 0$:

$$\langle p|\, e^{-\frac{i}{\hbar}\hat{H}\epsilon}\,|x\rangle=e^{-\frac{i}{\hbar}(\frac{p^2}{2m}+V(x))\epsilon}\,\langle p|x\rangle+\mathcal{O}(\epsilon^2). \tag{1.10}$$

We assume now that in the limit $\epsilon\to 0$, the higher order terms $\mathcal{O}(\epsilon^2)$ can be neglected[3]. Then,

$$\left\langle x'\right|\, e^{-\frac{i}{\hbar}\hat{H}\epsilon}\,|x\rangle\approx\int \mathrm{d}p\,\frac{1}{2\pi\hbar}e^{\frac{i}{\hbar}p(x'-x)}e^{-\frac{i\epsilon}{\hbar}(\frac{p^2}{2m}+V(x))}. \tag{1.11}$$

Now the integral is Gaussian and can be done:

$$\left\langle x'\right|\, e^{-\frac{i}{\hbar}\hat{H}\epsilon}\,|x\rangle\approx\frac{1}{2\pi\hbar}e^{-\frac{i\epsilon}{\hbar}V(x)}\int \mathrm{d}p\,e^{\frac{i}{\hbar}p(x'-x)-\frac{i\epsilon}{2m\hbar}p^2} \tag{1.12}$$

$$=\sqrt{\frac{m}{2\pi i\hbar\epsilon}}e^{\frac{i}{\hbar}\epsilon\left[\frac{1}{2}m\left(\frac{x'-x}{\epsilon}\right)^2-V(x)\right]}. \tag{1.13}$$

[2] We use the conventions: $\langle x|x'\rangle=\delta(x-x')$, $\langle p|p'\rangle=\delta(p-p')$ and $\langle x|p\rangle=\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px}$.

[3] see exercise 4 for more a detailed explanation

Now in the limit $\epsilon \to 0$,

$$\frac{x' - x}{\epsilon} \approx \dot{x} \tag{1.14}$$

$$\implies \epsilon \left[\frac{1}{2} m \left(\frac{x' - x}{\epsilon} \right)^2 - V(x) \right] \approx \epsilon \mathcal{L}(x, \dot{x}) \approx \int_0^\epsilon \mathrm{d}t \, \mathcal{L}(x, \dot{x}) = S(x', x) \tag{1.15}$$

Defining $\sqrt{\frac{m}{2\pi i \hbar \epsilon}} \equiv \frac{1}{A}$, we get

$$\left\langle x' \right| e^{-\frac{i}{\hbar} \hat{H} \epsilon} \left| x \right\rangle \approx \frac{1}{A} e^{\frac{i}{\hbar} S(x', x)}. \tag{1.16}$$

Using this result, we can go back to the propagator (eq 1.8):

$$K(x_f, t_f; x_i, t_i) = \int \mathrm{d}x_{N-1} \ldots \mathrm{d}x_1 \; \frac{1}{A^N} e^{\frac{i}{\hbar} \sum_{k=1}^{N} S(x_k, x_{k-1})} \tag{1.17}$$

At this point the limit $\epsilon \to 0$ can be taken:

$$K(x_f, t_f; x_i, t_i) = \lim_{\epsilon \to 0} \int \mathrm{d}x_{N-1} \ldots \mathrm{d}x_1 \; \frac{1}{A^N} e^{\frac{i}{\hbar} \sum_{k=1}^{N} S(x_k, x_{k-1})} \tag{1.18}$$

$$= \lim_{\epsilon \to 0} \frac{1}{A} \int \prod_{j=1}^{N-1} \frac{\mathrm{d}x_j}{A} \; e^{\frac{i}{\hbar} S[x(t)]} \tag{1.19}$$

$$\equiv \int_{\substack{x(t_i) = x_i \\ x(t_f) = x_f}} \mathcal{D}[x(t)] \; e^{\frac{i}{\hbar} S[x(t)]}, \tag{1.20}$$

where the action $S[x(t)]$ is

$$S[x(t)] = \int_{t_i}^{t_f} \mathrm{d}t \, \mathcal{L}(x, \dot{x}) \tag{1.21}$$

and the "path integral measure" $\mathcal{D}[x(t)]$ is **defined** as the limit $\epsilon \to 0$ of the product of integrals over the x_j's above. To summarize, we have an expression for the propagator in terms of a **path integral**:

$$\boxed{K(x_f, t_f; x_i, t_i) = \int_{\substack{x(t_i) = x_i \\ x(t_f) = x_f}} \mathcal{D}[x(t)] \; e^{\frac{i}{\hbar} S[x(t)]}} \tag{1.22}$$

This formula is the rigorous version of the formula (1.5) derived at the beginning when considering the double-slit experiment.

Example: Free Particle – As a first example, consider the case of a free particle, where

$$\mathcal{L}(x, \dot{x}) = \frac{1}{2} m \dot{x}^2. \tag{1.23}$$

Then

$$K(x_f,t,x_i,0)=\lim_{\epsilon\to 0}\frac{1}{A}\int\prod_{k=1}^{N-1}\frac{\mathrm{d}x_k}{A}\;e^{\frac{i}{\hbar}S}, \tag{1.24}$$

where

$$t=N\epsilon,\quad x_0=x_i,\ x_N=x_f,\quad S=\epsilon\sum_{k=1}^{N}\frac{1}{2}m\left(\frac{x_k-x_{k-1}}{\epsilon}\right)^2,\quad \frac{1}{A}=\sqrt{\frac{m}{2\pi i\hbar\epsilon}}$$

In order to do the integrals over the x_k's, we begin by doing the integral over x_1, then over x_2, and we will then see a pattern which will allow us to do all of them easily.

Each integration variables appears in two consecutive terms in the expression of S. For x_1, we have an integral of the following form:

$$\int_{-\infty}^{\infty}\mathrm{d}x_1\;e^{\frac{im}{2\hbar\epsilon}\left((x_1-x_0)^2+(x_2-x_1)^2\right)}=\frac{1}{\sqrt{2}}A\,e^{i\frac{m}{2\hbar\epsilon}\frac{(x_2-x_0)^2}{2}} \tag{1.25}$$

This term now enters the computation of the x_2 integral:

$$\int_{-\infty}^{\infty}\mathrm{d}x_2\;e^{i\frac{m}{2\hbar\epsilon}\left(\frac{(x_2-x_0)^2}{2}+(x_3-x_2)^2\right)}=\sqrt{\frac{2}{3}}Ae^{i\frac{m}{2\hbar\epsilon}\frac{(x_3-x_0)^2}{3}} \tag{1.26}$$

At this point we can see the pattern: the k-th integral will be

$$\int_{-\infty}^{\infty}\mathrm{d}x_k\;e^{i\frac{m}{2\hbar\epsilon}\left(\frac{(x_k-x_0)^2}{k}+(x_{k+1}-x_k)^2\right)}=\sqrt{\frac{k}{k+1}}Ae^{i\frac{m}{2\hbar\epsilon}\frac{(x_{k+1}-x_0)^2}{k+1}} \tag{1.27}$$

Therefore the propagator can be written

$$K(x_f,t,x_i,0)=\lim_{\epsilon\to 0}\frac{1}{A}\sqrt{\frac{1}{2}\frac{2}{3}\ldots\frac{N-1}{N}}e^{i\frac{m}{2\hbar\epsilon}\frac{(x_N-x_0)^2}{N}} \tag{1.28}$$

Taking the limit is trivial now as $N\epsilon=t$. In fact, in this simple example there is no need to take the limit. The correct answer is obtained for any finite N. We have obtained an explicit expression for the free propagator:

$$\boxed{K^{(\mathrm{free})}(x_f,t,x_i,0)=\sqrt{\frac{m}{2\pi i\hbar t}}\exp\left(i\frac{m}{2\hbar t}(x_f-x_i)^2\right)}. \tag{1.29}$$

Exercise 1.1 (The free propagator made easy)**.**
Compute the free propagator starting from

$$K^{(free)}(x_f,t,x_i,0)=\langle x_f|\,e^{-\frac{i}{\hbar}\hat{H}t}\,|x_i\rangle\,,\qquad \hat{H}=\frac{\hat{p}^2}{2m}\,, \tag{1.30}$$

and inserting the resolution of the identity in momentum eigenstates. Verify that your result matches the one obtained using the path integral formalism (equation 1.29).

Wavepacket evolution – The propagator can be used for computing the time evolution of wavepackets. Indeed,

$$\psi(x,t) = \langle x|\psi(t)\rangle = \langle x|\, e^{-\frac{i}{\hbar}\hat{H}t}\,|\psi(0)\rangle = \int \mathrm{d}y\ \langle x|\, e^{-\frac{i}{\hbar}\hat{H}t}\,|y\rangle\,\langle y|\psi(0)\rangle\,. \tag{1.31}$$

We recognize here the definition of the propagator, which leads to the useful formula

$$\boxed{\psi(x_f,t) = \int \mathrm{d}x_i\ K(x_f,t;x_i,0)\psi(x_i,0)}\,. \tag{1.32}$$

Exercise 1.2 (Gaussian wavepacket evolution)**.**

1. *Consider the following Gaussian wavefunction defined at $t = 0$:*

$$\psi(y,0) = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{\frac{i}{\hbar}py} e^{-\frac{y^2}{4\sigma^2}}. \tag{1.33}$$

Using formulas (1.32) and (1.29), verify that the wavefunction at time t is given by

$$\psi(x,t) = \frac{e^{-\frac{ip^2t}{2m\hbar}}}{(2\pi\sigma(t)^4/\sigma^2)^{1/4}} e^{\frac{i}{\hbar}px} e^{-\left(x-\frac{p}{m}t\right)^2/4\sigma(t)^2}, \tag{1.34}$$

where

$$\sigma(t)^2 = \sigma^2 + i\frac{\hbar t}{2m} \tag{1.35}$$

2. *Compute $|\psi(x,t)|^2$ and read off the average position $\langle x\rangle$ and the width $\left\langle (x-\langle x\rangle)^2\right\rangle$ of the particle as a function of time. Comment on your results.*
Hint: the standard form of a Gaussian distribution is

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \tag{1.36}$$

where μ is the mean and σ^2 is the standard deviation.

3. *Rederive the previous results in momentum space:*

$$\psi(x,t) = \int dk\ \langle x|\, e^{-\frac{i}{\hbar}\hat{H}t}\,|k\rangle\,\langle k|\psi(0)\rangle\,. \tag{1.37}$$

The phase space path integral

The phase space path integral is what we obtain if we do not perform the gaussian integral in p during the derivation of the path integral formulation. Explicitly, we use equations (1.8) and (1.11) to get

$$\begin{aligned} K(x_f,T;x_i,0) &= \int \mathrm{d}x_{N-1}\ldots\mathrm{d}x_1 \prod_{k=1}^{N}\left(\int \frac{\mathrm{d}p_k}{2\pi\hbar} e^{\frac{i\epsilon}{\hbar}\left[p\frac{x_k-x_{k-1}}{\epsilon}-(\frac{p^2}{2m}+V(x))\right]}\right), \quad (T=N\epsilon) \\ &= \int \frac{\mathrm{d}p_N}{2\pi\hbar}\prod_{k=1}^{N-1}\left(\int \frac{\mathrm{d}x_k\mathrm{d}p_k}{2\pi\hbar}\right) e^{\frac{i}{\hbar}\int_0^T \mathrm{d}t\,[p\dot{x}-H(p,x)]} \\ &\equiv \int_{\substack{x(0)=x_i \\ x(T)=x_f}} \mathcal{D}[x(t)]\mathcal{D}[p(t)] e^{\frac{i}{\hbar}S[x(t),p(t)]} \end{aligned} \tag{1.38}$$

It may help to draw the real space trajectory and the momentum space trajectory in the same picture (1.6). There is a momentum integral for each time step, which is why they are represented in between each position integral.

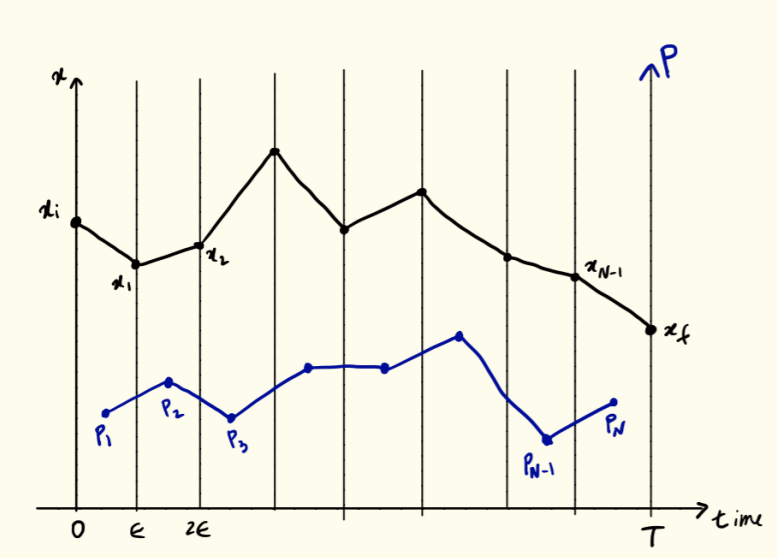


Figure 1.6

Some properties of the propagator

Note first that

$$\begin{aligned} K(x_f,t_f;x_i,t_i) &= \langle x_f|\, e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}\,|x_i\rangle \\ &= \int \mathrm{d}x_m\ \langle x_f|\, e^{-\frac{i}{\hbar}\hat{H}(t_f-t)}\,|x_m\rangle\,\langle x_m|\, e^{-\frac{i}{\hbar}\hat{H}(t-t_i)}\,|x_i\rangle \\ &= \int \mathrm{d}x_m\ K(x_f,t_f;x_m,t_m)K(x_m,t_m;x_i,t_i). \end{aligned} \tag{1.39}$$

This **composition property** follows directly from the path integral representation:

$$K(x_f, t_f; x_i, t_i) = \int_{\substack{x(t_i)=x_i \\ x(t_f)=x_f}} \mathcal{D}[x(t)] e^{\frac{i}{\hbar} S[x(t)]} \tag{1.40}$$

$$= \int \mathrm{d}x_m \int_{\substack{x(t_i)=x_i \\ x(t_m)=x_m}} \mathcal{D}[x_1(t)] \int_{\substack{x(t_m)=x_m \\ x(t_f)=x_f}} \mathcal{D}[x_2(t)] e^{\frac{i}{\hbar}(S[x_1(t)]+S[x_2(t)])} \tag{1.41}$$

$$= \int \mathrm{d}x_m \; K(x_f, t_f; x_m, t_m) K(x_m, t_m; x_i, t_i), \tag{1.42}$$

This result can be understood easily by drawing the trajectory as in figure (1.7)

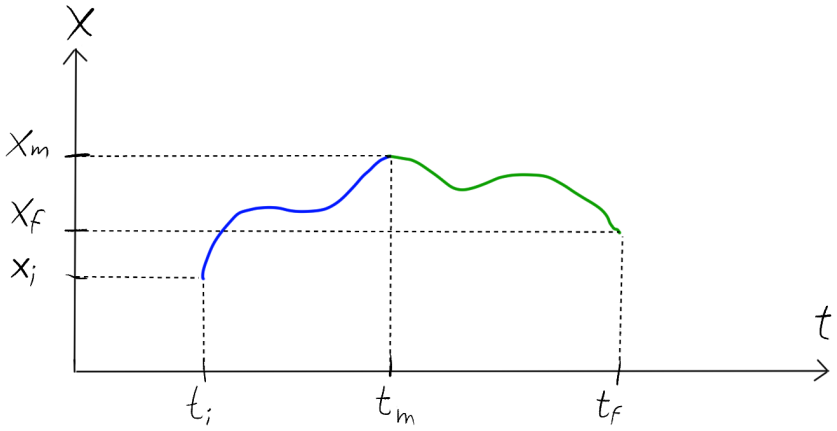


Figure 1.7: Illustration of the composition property of the path integral

One can also derive a **differential equation for the propagator**. Let

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t} |x_0\rangle .$$

Then,

$$K(x, t; x_0, 0) = \langle x|\psi(t)\rangle = \psi(x, t)$$
$$\implies K(x, t; x_0, 0) \text{ solves the Schrödinger equation for the variables } x, t$$

Furthermore, the propagator verifies a boundary condition in time:

$$\lim_{t\to 0} K(x, t; x_0, 0) = \langle x|x_0\rangle = \delta(x - x_0). \tag{1.43}$$

These two properties fix the propagator uniquely.

Summary of Lecture 1

- Path integral representation of the propagator:

$$K(x_f, t; x_i, 0) = \langle x_f | \, e^{-\frac{i}{\hbar}\hat{H}t} \, | x_i \rangle = \int_{\substack{x(t_i)=x_i \\ x(t_f)=x_f}} \mathcal{D}[x(t)] \; e^{\frac{i}{\hbar}S[x(t)]}$$

- Free particle propagator:

$$K^{(\text{free})}(x_f, t, x_i, 0) = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(i\frac{m}{2\hbar t}(x_f - x_i)^2\right)$$

Lecture 2 - Gaussian path integrals

"The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing levels of abstraction" - Sydney Coleman

Now that we have defined the path integral for a general action, our first goal is to compute it for the harmonic oscillator. The action of the harmonic oscillator is quadratic in x, which is why we first study generic **Gaussian** integrals, and then move on to the full path integral of the HO.

Gaussian integrals

The goal is to eventually be able to compute the propagator of the harmonic oscillator. To do so, we first review regular gaussian integrals. It is well known that in 1 dimension,

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-\lambda x^2} = \sqrt{\frac{\pi}{\lambda}}, \quad \lambda > 0 \tag{1.44}$$

Consider now the generalization to the n-dimensional Gaussian integral:

$$I_n \equiv \int \mathrm{d}^n\mathbf{x}\, e^{-\mathbf{x}^T\Lambda\mathbf{x}}, \quad \Lambda \in M_{n\times n}, \quad \Lambda^T = \Lambda \tag{1.45}$$

Exercise 1.3.
Argue why we do not need to consider the more general case where $\Lambda^T \neq \Lambda$. Hint: any matrix M can be decomposed into its symmetric and antisymmetric parts as

$$M = \frac{1}{2}(M + M^T) + \frac{1}{2}(M - M^T)$$

Since Λ is symmetric, it can be diagonalized using an orthogonal matrix O (this is the spectral theorem):

$$O^T\Lambda O = \mathrm{diag}(\lambda_1, \ldots, \lambda_n), \quad O^TO = \mathbb{1}, \quad \det(O) = \pm 1 \tag{1.46}$$

In order to evaluate I_n, we perform a change of variable using this orthogonal matrix: $\mathbf{x} = O\mathbf{y}$. Then

$$I_n \equiv \int \mathrm{d}^n\mathbf{y}\, \underbrace{|\det(O)|}_{=1} e^{-\mathbf{y}^TO^T\Lambda O\mathbf{y}} = \int \mathrm{d}^n\mathbf{y}\, e^{-\sum_{i=1}^n \lambda_i y_i^2} = \prod_{i=1}^n \sqrt{\frac{\pi}{\lambda_i}}. \tag{1.47}$$

Therefore,

$$\boxed{\int \mathrm{d}^n\mathbf{x}\, e^{-\mathbf{x}^T\Lambda\mathbf{x}} = \frac{\pi^{n/2}}{\sqrt{\det(\Lambda)}}}. \tag{1.48}$$

One might wonder what happens if $\det(\Lambda) \leq 0$. This is not real cause for concern as it would mean that at least one of the λ_i is less than or equal to 0, and therefore the integral I_n would diverge.

After considering n-dimensional *real* gaussian integrals, we look at *complex* gaussian integrals. Consider

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{i\lambda x^2}, \quad \lambda \in \mathbb{R} \tag{1.49}$$

A possible way to compute this integral is to analytically continue the real result (1.44). To do so, we start with a real number $\alpha > 0$ and rotate it in the complex plane (see figure 1.8) so that it lands at $\pm i\alpha$.

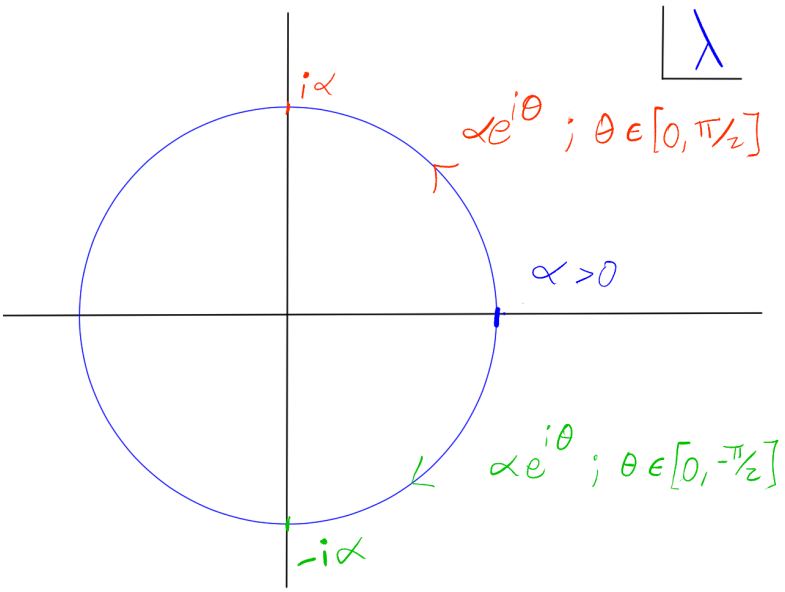


Figure 1.8: Rotations by $\pm\pi/2$ in the complex plane

Using this operation, we can get the complex integral from the real one. Consider the transformation $\alpha \to -i\alpha$:

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-\alpha x^2} \to \int_{-\infty}^{\infty} \mathrm{d}x\, e^{i\alpha x^2}, \quad \alpha > 0 \tag{1.50}$$

Now we have to analytically continue the right-hand side:

$$\sqrt{\frac{\pi}{\alpha}} = \sqrt{\frac{\pi}{\alpha e^{-i\pi/2}}} = e^{i\pi/4}\sqrt{\frac{\pi}{\alpha}} \tag{1.51}$$

We therefore have our result (check the case $\alpha \to i\alpha$ for the other sign possibility):

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{i\lambda x^2} = e^{i\,\mathrm{sgn}(\lambda)\pi/4}\sqrt{\frac{\pi}{|\lambda|}} \tag{1.52}$$

This result can also be obtained by methods of complex analysis involving contour integrals (see exercise 1 in the appendix).

Using the same reasoning as for the n-dimensional real Gaussian integral, we find the n-dimensional complex Gaussian integral:

$$\boxed{\int \mathrm{d}^n\mathbf{x}\, e^{i\mathbf{x}^T\Lambda\mathbf{x}} = e^{i(n_+-n_-)\pi/4}\frac{\pi^{n/2}}{\sqrt{|\det(\Lambda)|}}}, \tag{1.53}$$

where $n_\pm$ is the number of positive (negative) eigenvalues of Λ.

The harmonic oscillator path integral

Consider now the harmonic oscillator propagator:

$$K(x_f,t_f;x_i,t_i) = \int_{\substack{x(t_i)=x_i\\x(t_f)=x_f}} \mathcal{D}[x(t)]e^{\frac{i}{\hbar}S[x(t)]}, \tag{1.54}$$

$$\text{where } S[x(t)] = \int_{t_i}^{t_f}\mathrm{d}t\,\left(\frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2\right). \tag{1.55}$$

We can find the classical trajectory $x_c(t)$ easily:

$$\ddot{x}_c(t)+\omega^2x_c(t)=0\,,\qquad x_c(t_i)=x_i\,,\qquad x_c(t_f)=x_f\,.$$

Consider now the change of variables $x(t)=x_c(t)+y(t)$. The boundary conditions of the path integral now change to $y(t_i)=y(t_f)=0$, but the measure does not since the change of variables is linear: $\mathcal{D}[x(t)]=\mathcal{D}[y(t)]$. We get

$$K(x_f,t_f;x_i,t_i) = \int_{\substack{y(t_i)=0\\y(t_f)=0}} \mathcal{D}[y(t)]e^{\frac{i}{\hbar}S[x_c(t)+y(t)]}. \tag{1.56}$$

Let us now see what happens with the action.

$$S[x_c(t)+y(t)] = \int_{t_i}^{t_f}\mathrm{d}t\,\frac{1}{2}m(\dot{x}_c+\dot{y})^2 - \frac{1}{2}m\omega^2(x_c+y)^2 \tag{1.57}$$

$$= S[x_c(t)] + S[y(t)] + m\int_{t_i}^{t_f}\mathrm{d}t\,\dot{x}_c\dot{y} - \omega^2x_cy \tag{1.58}$$

$$= S[x_c(t)] + S[y(t)] - m\int_{t_i}^{t_f}\mathrm{d}t\,y(t)(\underbrace{\ddot{x}_c+\omega^2x_c}_{=0\ \text{(E.O.M.)}}) \tag{1.59}$$

This is not a coincidence! Indeed,

$$S[x_c+y] = S[x_c] + \int \mathrm{d}t \quad \underbrace{\frac{\delta S}{\delta x(t)}}_{=0 \text{ (E.O.M.)}} \Bigg|_{x=x_c} y(t) + \frac{1}{2}\iint \mathrm{d}t_1\mathrm{d}t_2 \, \frac{\delta^2 S}{\delta x(t_1)\delta x(t_2)}\Bigg|_{x=x_c} y(t_1)y(t_2) + \frac{1}{3!}\iiint \mathrm{d}t_1\mathrm{d}t_2\mathrm{d}t_3 \, \underbrace{\frac{\delta^3 S}{\delta x(t_1)\delta x(t_2)\delta x(t_3)}}_{=0 \text{ (quadratic action)}}\Bigg|_{x=x_c} y(t_1)y(t_2)y(t_3) + \dots$$

With this result in hand, we can see that the propagator can be written as

$$K(x_f,t_f;x_i,t_i) = e^{\frac{i}{\hbar}S[x_c(t)]} \int_{\substack{y(t_i)=0\\ y(t_f)=0}} \mathcal{D}[y(t)] e^{\frac{i}{\hbar}S[y(t)]} \tag{1.60}$$

$$= e^{\frac{i}{\hbar}S[x_c(t)]} K(0,t_i;0,t_f) \tag{1.61}$$

$$\equiv e^{\frac{i}{\hbar}S[x_c(t)]} J(t_f-t_i), \tag{1.62}$$

where we can write $K(0,t_i;0,t_f) \equiv J(t_f-t_i)$ thanks to time translation symmetry.

Exercise 1.4 (Classical action of the Harmonic Oscillator)**.**
Show that

$$S[x_c] = \frac{m\omega}{2}\frac{\left(x_f^2+x_i^2\right)\cos(\omega T) - 2x_i x_f}{\sin(\omega T)}, \quad T = t_f - t_i\,. \tag{1.63}$$

What is left to compute is the function $J(T)$. The first step is to rewrite the integrand in a form comparable to a Gaussian integral (similar to 1.48):

$$S[y] = \int_0^T \mathrm{d}t \, \left(\frac{1}{2}m\dot{y}^2 - \frac{1}{2}m\omega^2 y^2\right) = \frac{m}{2}\int_0^T \mathrm{d}t \, y \underbrace{\left(-\frac{\mathrm{d}^2}{\mathrm{d}t^2} - \omega^2\right)}_{\equiv \hat{O}} y \tag{1.64}$$

$$\implies J(T) = \int_{\substack{y(t_i)=0\\ y(t_f)=0}} \mathcal{D}[y(t)] e^{\frac{i}{\hbar}\frac{m}{2}\int_0^T \mathrm{d}t \, y\hat{O}y} \tag{1.65}$$

By analogy with the n-dimensional Gaussian integral, we expect $J(T) \propto |\det \hat{O}|^{-1/2}$. More explicitly, we can expand the integration variable $y(t)$ in a complete basis of orthonormal eigenfunctions of the operator $\hat{O}$. This is the equivalent of diagonalizing the matrix Λ in the n-dimensional case.

Define the eigenfunctions $y_n(t)$ as

$$\hat{O}y_n(t) = \lambda_n y_n(t), \quad y_n(0) = y_n(T) = 0$$
$$\implies y_n(t) = \sqrt{\frac{2}{T}} \sin\left(\frac{n\pi t}{T}\right), \quad \lambda_n = \left(\frac{n\pi}{T}\right)^2 - \omega^2$$

Here, we chose to normalize the eigenfunctions by $\int_0^T dt (y_n(t))^2 = 1$. Note that the sign of λ_n depends on how big n is. For small n, $\lambda_n < 0$, but for $n > \frac{\omega T}{\pi}$, $\lambda_n > 0$. Therefore, the number of negative eigenvalues of $\hat{O}$ is $n_- = \text{int}\left(\frac{\omega T}{\pi}\right)$.[4]

We can now expand $y(t)$ in the complete basis given by the $y_n(t)$:

$$y(t) = \sum_{n=1}^{\infty} a_n y_n(t) \tag{1.66}$$

Since the $y_n(t)$ are fixed now, it makes sense that we have to integrate over the coefficients a_n. Since we are changing variables, we need to keep track of the jacobian, which we denote $\tilde{N}$. It is important to notice that since the eigenfunctions $y_n(t)$ do not depend on ω, neither does the jacobian $\tilde{N}$. Furthermore, for reasons that will become clear soon, it is convenient to pull out a factor $\frac{1}{\sqrt{2\pi i}}$ from the jacobian for each a_n, such that the path integral measure becomes

$$\mathcal{D}[y] \to \int \prod_n \frac{\mathrm{d}a_n}{\sqrt{2\pi i}} \tilde{N}. \tag{1.67}$$

In terms of the new variables a_n, we have

$$\int_0^T \mathrm{d}t\, y\hat{O}y = \int_0^T \mathrm{d}t \sum_{n,m} a_n a_m y_n(t) \hat{O} y_m(t) \tag{1.68}$$
$$= \sum_{n,m} a_n a_m \lambda_m \underbrace{\int_0^T \mathrm{d}t\, y_n(t) y_m(t)}_{\delta_{n,m}} \tag{1.69}$$
$$= \sum_n a_n^2 \lambda_n. \tag{1.70}$$

The path integral therefore becomes a product of gaussian integrals that we can evaluate:

$$J(T) = \int \left(\prod_n \frac{\mathrm{d}a_n}{\sqrt{2\pi i}}\right) \tilde{N} e^{\frac{i}{\hbar}\frac{m}{2}\sum_n a_n^2 \lambda_n} = \tilde{N} \frac{e^{i\frac{\pi}{4}(n_+ - n_-)}}{(2\pi i)^{\frac{1}{2}(n_+ + n_-)}} \prod_n \sqrt{\frac{2\pi\hbar}{m|\lambda_n|}} \tag{1.71}$$
$$= \tilde{N} \underbrace{\frac{e^{i\frac{\pi}{4}(n_+ - n_-)}}{e^{i\frac{\pi}{4}(n_+ + n_-)}}}_{= e^{-i\frac{\pi}{2}n_-}} \prod_n \sqrt{\frac{\hbar}{m|\lambda_n|}} \tag{1.72}$$

[4] The function $\text{int}(x)$ gives the largest integer smaller or equal than x.

Now you might be worried that the product $\prod_n \sqrt{\frac{\hbar}{m|\lambda_n|}}$ is identically 0, since we have an infinite product of smaller and smaller numbers (the λ_n grow as n^2). However, the product of the $\tilde{N}$ with $\prod_n \sqrt{\frac{\hbar}{m|\lambda_n|}}$ is finite and well defined. [5] Indeed, we can take a **ratio** of two functions $J(T)$ with different values of ω. This is useful because, as we mentioned before, the jacobian $\tilde{N}$ does not depend on ω and cancels out when we take the ratio. We therefore compute:

$$\frac{J_\omega(T)}{J_0(T)} = \frac{\tilde{N}e^{-i\frac{\pi}{2}n_-(\omega)}\prod_n \sqrt{\frac{\hbar}{m|\lambda_n(\omega)|}}}{\tilde{N}e^{-i\frac{\pi}{2}n_-(0)}\prod_n \sqrt{\frac{\hbar}{m|\lambda_n(0)|}}} \tag{1.74}$$

$$= e^{-i\frac{\pi}{2}(n_-(\omega)-n_-(0))}\left|\frac{\det \hat{O}_\omega}{\det \hat{O}_0}\right|^{-1/2} \tag{1.75}$$

Since $n_-(0) = 0$, we write $n_- \equiv n_-(\omega)$. Furthermore, the ratio of determinants can be computed as

$$\frac{\det \hat{O}_\omega}{\det \hat{O}_0} = \prod_{n=1}^{\infty} \frac{\left(\frac{n\pi}{T}\right)^2 - \omega^2}{\left(\frac{n\pi}{T}\right)^2} = \prod_{n=1}^{\infty}\left[1 - \left(\frac{\omega T}{n\pi}\right)^2\right] \tag{1.76}$$

This expression has zeros at $\omega T = n\pi$, just like a sine function. However, as $\omega T \to 0$, the ratio of determinants tends to 1. Moreover, it does not have any poles. We can therefore guess that

$$\frac{\det \hat{O}_\omega}{\det \hat{O}_0} = \frac{\sin(\omega T)}{\omega T} \tag{1.77}$$

This qualitative reasoning can be made rigorous by using the Weierstrass factorization theorem[6]. All the pieces needed to conclude the derivation are present: we have

$$J_\omega(T) = e^{-i\frac{\pi}{2}n_-}\sqrt{\frac{\omega T}{|\sin(\omega T)|}}\sqrt{\frac{m}{2\pi i\hbar T}}, \tag{1.78}$$

where we used the expression for the free propagator found in lecture 1 (equation 1.29), since $J_0(T) = K^{(\text{free})}(0, T; 0, 0)$. Having found $J_\omega(T)$, we finally put everything together to obtain **the harmonic oscillator propagator**:

$$\boxed{K^{(\text{HO})}(x_f, T; x_i, 0) = e^{-i\frac{\pi}{2}\,\text{int}\left(\frac{\omega T}{\pi}\right)}\sqrt{\frac{m\omega}{2\pi i\hbar|\sin(\omega T)|}}e^{i\frac{m\omega}{2\hbar}\frac{\left(x_f^2+x_i^2\right)\cos(\omega T)-2x_i x_f}{\sin(\omega T)}}}. \tag{1.79}$$

[5] A more careful approach to this problem would be to go back to the definition of the path integral with discretized time, and take the limit $\epsilon \to 0$ at the end of the computation. If

$$\int_{\substack{y(0)=0\\y(T)=0}} \mathcal{D}[y(t)] \to \lim_{\epsilon\to 0}\frac{1}{A}\int\prod_{j=1}^{N-1}\frac{\mathrm{d}y_j}{A}, \tag{1.73}$$

then the operator $\hat{O}$ becomes a finite matrix. We will take this approach in the next lecture.

[6] `https://en.wikipedia.org/wiki/Weierstrass_factorization_theorem`

Summary of Lecture 2

- Gaussian integrals

$$\int \mathrm{d}^n\mathbf{x}\, e^{-\mathbf{x}^T\Lambda\mathbf{x}} = \frac{\pi^{n/2}}{\sqrt{\det(\Lambda)}}$$
$$\int \mathrm{d}^n\mathbf{x}\, e^{i\mathbf{x}^T\Lambda\mathbf{x}} = e^{i(n_+-n_-)\pi/4}\frac{\pi^{n/2}}{\sqrt{|\det(\Lambda)|}}$$

- Harmonic Oscillator

$$K^{(\mathrm{HO})}(x_f,T;x_i,0) = e^{\frac{i}{\hbar}S[x_c]}\int_{\substack{y(0)=0\\y(T)=0}}\mathcal{D}[y]\, e^{\frac{i}{\hbar}S[y]} \quad (x = x_c + y)$$
$$= e^{-i\frac{\pi}{2}\,\mathrm{int}\left(\frac{\omega T}{\pi}\right)}\sqrt{\frac{m\omega}{2\pi i\hbar|\sin(\omega T)|}}\, e^{i\frac{m\omega}{2\hbar}\frac{\left(x_f^2+x_i^2\right)\cos(\omega T)-2x_ix_f}{\sin(\omega T)}}$$

Lecture 3 - Gelfand-Yaglom formula and time-ordered products

Time-dependent harmonic oscillator

Consider the time dependent harmonic oscillator:

$$\mathcal{L} = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2(t)x^2 \tag{1.80}$$

Following the same method as for the time-independent harmonic oscillator, we can write the propagator as

$$K(x_f, t_f; x_i, t_i) = e^{\frac{i}{\hbar}S[x_c]}K(0, t_f; 0, t_i), \tag{1.81}$$

where $x_c(t)$ is the classical solution (we used the change of variables $x(t) = x_c(t) + y(t)$).

In order to make progress, we use the definition of the path integral as a limit $N \to \infty$ of the system with discretized time. Let

$$t_i \equiv t_0,\ t_f \equiv t_{N+1}, \quad \epsilon = \frac{t_f - t_i}{N+1}, \quad \omega_j \equiv \omega(t_j) \tag{1.82}$$

We use this convention so that there are $N+1$ time steps and N integrals (over $y_1, \ldots, y_N$):

$$K(0, t_f; 0, t_i) = \lim_{N\to\infty} \int \mathrm{d}y_1 \ldots \mathrm{d}y_N \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N+1}{2}} e^{\frac{i}{\hbar}\sum_{j=0}^{N}\frac{m}{2}\epsilon\left[\left(\frac{y_{j+1}-y_j}{\epsilon}\right)^2 - \omega_j^2 y_j^2\right]} \tag{1.83}$$

At this point it is convenient to define:

$$\mathbf{y} \equiv \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, \quad \sigma = \frac{m}{2\hbar\epsilon}\tilde{\sigma} \tag{1.84}$$

$$\tilde{\sigma} \equiv \begin{pmatrix} 2 & -1 & 0 & \ldots & & 0 \\ -1 & 2 & -1 & & & \\ 0 & -1 & 2 & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & & \\ & & & & 2 & -1 \\ 0 & & \ldots & & -1 & 2 \end{pmatrix} - \epsilon^2 \begin{pmatrix} \omega_1^2 & & & \ldots & & 0 \\ & \omega_2^2 & & & & \\ & & \omega_3^2 & & & \vdots \\ \vdots & & & \ddots & & \\ & & & & \omega_{N-1}^2 & \\ 0 & & \ldots & & & \omega_N^2 \end{pmatrix} \tag{1.85}$$

With these definitions in hand, we can write the propagator as

$$K(0, t_f; 0, t_i) = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N+1}{2}} \int \mathrm{d}^N\mathbf{y} e^{i\mathbf{y}^T\sigma\mathbf{y}} \tag{1.86}$$

Now the integral can be computed using equation (1.53) to get

$$K(0,t_f;0,t_i) = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N+1}{2}} e^{i(n_+-n_-)\frac{\pi}{4}}\frac{\pi^{N/2}}{\sqrt{|\det(\sigma)|}} \tag{1.87}$$

$$= \lim_{N\to\infty} e^{i(n_+-n_-)\frac{\pi}{4}}\left[\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N+1}\frac{\pi^N}{|\det(\sigma)|}\right]^{1/2} \tag{1.88}$$

$$= \lim_{N\to\infty}\sqrt{\frac{m}{2\pi i\hbar}}e^{i(n_+-n_-)\frac{\pi}{4}}\left[\left(\frac{1}{i}\right)^{N}\frac{1}{\epsilon|\det(\tilde{\sigma})|}\right]^{1/2} \tag{1.89}$$

$$= \lim_{N\to\infty}\sqrt{\frac{m}{2\pi i\hbar}}e^{-i\frac{\pi}{2}n_-}\left[\frac{1}{\epsilon|\det(\tilde{\sigma})|}\right]^{1/2} \tag{1.90}$$

where we used $\det(\sigma) = \left(\frac{m}{2\hbar\epsilon}\right)^N \det(\tilde{\sigma})$ and $i^{-1/2} = e^{-i\frac{\pi}{4}}$. Note that the result depends on n_-, the number of negative eigenvalues of σ. In the continuum limit, the size of σ is sent to infinity, and we can interpret n_- in a different way. To do so, recall that originally we had

$$K(0,t_f;0,t_i) = \int \mathcal{D}[y(t)]e^{\frac{i}{\hbar}\int_{t_i}^{t_f}\frac{1}{2}m\dot{y}^2-\frac{1}{2}m\omega^2(t)y^2} \tag{1.91}$$

$$= \int \mathcal{D}[y(t)]e^{\frac{im}{2\hbar}\int_{t_i}^{t_f} y\left(-\frac{\mathrm{d}^2}{\mathrm{d}t^2}-\omega^2(t)\right)y} \tag{1.92}$$

where we integrated by parts and used $y(t_i) = y(t_f) = 0$. In the above, one can identify $-\frac{\mathrm{d}^2}{\mathrm{d}t^2} - \omega^2(t)$ as the $N\to\infty$ analog of $\tilde{\sigma}$ by comparison with (1.86) [7]. We can therefore interpret n_- as the number of negative eigenvalues of the operator $-\frac{\mathrm{d}^2}{\mathrm{d}t^2} - \omega^2(t)$.

Now that we understand n_- in the $N\to\infty$ limit, our task is to compute $\det(\tilde{\sigma})$. To do so, we compute the determinant by the Laplace method (also known as cofactor method). Define p_j as the determinant of the top left $j\times j$ block of $\tilde{\sigma}$:

$$p_j = \det[\tilde{\sigma}]_{j\times j} \tag{1.93}$$

Then,

$$p_1 = 2-\epsilon^2\omega_1^2 \tag{1.94}$$

$$p_2 = (2-\epsilon^2\omega_1^2)(2-\epsilon^2\omega_2^2) - 1 \tag{1.95}$$

$$\vdots$$

$$p_{j+1} = \det\left(\begin{array}{ccc|c} & \tilde{\sigma}_{j\times j} & & \begin{array}{c}0\\ \vdots\\ -1\end{array} \\ \hline 0 & \cdots & -1 & 2-\epsilon^2\omega_{j+1}^2 \end{array}\right) \tag{1.96}$$

[7] Since we only care about the number of negative eigenvalues n_-, the overall factors of m or $\hbar$ are irrelevant - there is therefore no difference between n_- for σ or for $\tilde{\sigma}$.

We can now write p_{j+1} as a function of p_j using the method of cofactors. We develop the determinant along the last column to get:

$$p_{j+1} = \det \left(\begin{array}{ccccc|c} & & & & 0 & 0 \\ & \tilde{\sigma}_{j-1\times j-1} & & & \vdots & \vdots \\ & & & & -1 & 0 \\ 0 & \dots & -1 & 2-\epsilon^2\omega_j^2 & & -1 \\ \hline 0 & \dots & 0 & -1 & & 2-\epsilon^2\omega_{j+1}^2 \end{array} \right) \tag{1.97}$$

$$= (2-\epsilon^2\omega_{j+1}^2)p_j - (-1)\cdot \det \left(\begin{array}{ccc|c} & \tilde{\sigma}_{j-1\times j-1} & & \begin{array}{c} 0 \\ \vdots \\ -1 \end{array} \\ \hline 0 & \cdots\cdots & 0 & -1 \end{array} \right) \tag{1.98}$$

$$= (2-\epsilon^2\omega_{j+1}^2)p_j - p_{j-1}, \tag{1.99}$$

where in the last line we developed the determinant along the last row. This procedure gives us a recurrence equation on the p_j's:

$$\frac{p_{j+1} - 2p_j + p_{j-1}}{\epsilon^2} = -\omega_{j+1}^2 p_j \tag{1.100}$$

As $\epsilon \to 0$, this becomes a differential equation! Indeed, define

$$\epsilon p_j \equiv \varphi(t_i + \epsilon\cdot j), \quad j = 1, \dots, N. \tag{1.101}$$

Then, equation (1.100) implies

$$\frac{\varphi(t_i+\epsilon(j+1)) - 2\varphi(t_i+\epsilon\cdot j) + \varphi(t_i+\epsilon(j-1))}{\epsilon^2} = -\omega_{j+1}^2\varphi(t_i+\epsilon\cdot j) \tag{1.102}$$

$$\implies \ddot{\varphi}(t) = -\omega^2(t)\varphi(t). \tag{1.103}$$

The initial conditions are given by

$$\varphi(t_i) = \lim_{\epsilon\to 0} \epsilon p_1 = 0 \tag{1.104}$$

$$\dot{\varphi}(t_i) = \lim_{\epsilon\to 0} \frac{\epsilon p_2 - \epsilon p_1}{\epsilon} = 1 \tag{1.105}$$

Therefore, given the time-dependent frequency $\omega(t)$, one can solve for $\varphi(t)$. What is relevant to us is to compute

$$\lim_{N\to\infty} \epsilon \det(\tilde{\sigma}) = \lim_{N\to\infty} \epsilon p_N = \varphi(t_f) \tag{1.106}$$

This gives us an expression for the time-dependent harmonic oscillator propagator:

$$\boxed{K(x_f,t_f;x_i,t_i) = e^{\frac{i}{\hbar}S[x_c]} e^{-i\frac{\pi}{2}n_-} \sqrt{\frac{m}{2\pi i\hbar|\varphi(t_f)|}}}, \tag{1.107}$$

where $\varphi(t)$ is the solution to the following ODE:

$$\ddot{\varphi}(t) = -\omega^2(t)\varphi(t), \quad \begin{cases} \varphi(t_i) = 0 \\ \dot{\varphi}(t_i) = 1 \end{cases} \tag{1.108}$$

Equation (1.107) is known as the **Gelfand-Yaglom formula**. At first it is surprising to realize that we have found an analytic expression for the propagator of the time-dependent harmonic oscillator. However, path integrals with quadratic actions are in a sense a generalization of Gaussian integrals, so we expect to be able to solve them exactly.

Exercise 1.5.
Use the Gelfand-Yaglom formula to re-derive the propagators for the free particle ($\omega = 0$) and the harmonic oscillator ($\omega = const$).

Operator matrix elements

Recall that in the Schrödinger picture, the states $|\psi(t)\rangle$ evolve in time while the operators $\hat{O}$ are fixed. In the Heisenberg picture, the states $|\psi\rangle$ are fixed and the operators $\hat{O}(t)$ evolve. To go from one picture to another, we use the formula

$$\hat{O}_H(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{O}_S e^{-\frac{i}{\hbar}\hat{H}t}. \tag{1.109}$$

Define now the state $|x,t\rangle$ as an eigenstate of the (Heisenberg picture) position operator $\hat{x}(t)$. We can write this state in terms of the $|x\rangle$, the eigenstate of the (Schrödinger picture) operator $\hat{x}$ as follows:

$$\begin{aligned} |x,t\rangle &\equiv e^{\frac{i}{\hbar}\hat{H}t}|x\rangle \quad \text{(this is } \textit{not} \text{ time evolution!)} \\ \implies \hat{x}(t)|x,t\rangle &= \left(e^{\frac{i}{\hbar}\hat{H}t}\hat{x}e^{-\frac{i}{\hbar}\hat{H}t}\right)e^{\frac{i}{\hbar}\hat{H}t}|x\rangle = x|x,t\rangle \end{aligned}$$

Then, we can write the propagator in terms of the $|x,t\rangle$:

$$\langle x_f,t_f|x_i,t_i\rangle = \langle x_f|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|x_i\rangle = K(x_f,t_f;x_i,t_i) = \int \mathcal{D}[x]e^{\frac{i}{\hbar}S[x]}$$

You may have noticed that the path integral representation of the propagator is similar to the kind of expressions one gets in statistical mechanics:

$$\begin{aligned} Z &= \sum_{\text{config}} e^{-\beta H} \\ \langle\mathcal{O}\rangle &= \frac{1}{Z}\sum_{\text{config}} \mathcal{O}e^{-\beta H}, \end{aligned}$$

if we identify $-\beta H$ with $\frac{i}{\hbar}S$. This leads us to wonder about the possible physical significance of an expression such as:

$$\int \mathcal{D}[x]\, A(x(t_1))e^{\frac{i}{\hbar}S[x]}, \quad t_i < t_1 < t_f, \tag{1.110}$$

where $A = A(x)$ is some function of x. It seems intuitive to use the composition property (1.39) to break up the path integral into two regions: the first region where the particle evolves from t_i to t_1 (labelled by a), and the second where it evolves from t_1 to t_f (labelled by b). We can then write

$$\begin{aligned}
\int \mathcal{D}[x]\, e^{\frac{i}{\hbar}S[x]} A(x(t_1)) &= \int \mathrm{d}x_1 \int_{\substack{x_a(t_i)=x_i \\ x_a(t_1)=x_1}} \mathcal{D}[x_a] \int_{\substack{x_b(t_1)=x_1 \\ x_b(t_f)=x_f}} \mathcal{D}[x_b]\, e^{\frac{i}{\hbar}(S_a+S_b)} A(x_1) \\
&= \langle x_f|\, e^{-\frac{i}{\hbar}\hat{H}(t_f-t_1)} \underbrace{\int \mathrm{d}x_1\, |x_1\rangle\, A(x_1)\, \langle x_1|}_{=A(\hat{x})}\, e^{-\frac{i}{\hbar}\hat{H}(t_1-t_i)}\, |x_i\rangle \\
&= \langle x_f|\, e^{-\frac{i}{\hbar}\hat{H}t_f} \underbrace{e^{\frac{i}{\hbar}\hat{H}t_1} A(\hat{x}) e^{-\frac{i}{\hbar}\hat{H}t_1}}_{=A(\hat{x}(t_1))}\, e^{\frac{i}{\hbar}\hat{H}t_i}\, |x_i\rangle \\
&= \langle x_f, t_f|\, A(\hat{x}(t_1))\, |x_i, t_i\rangle
\end{aligned}$$

Therefore we see that we have

$$\begin{aligned}
\langle x_f, t_f | x_i, t_i\rangle &= \int \mathcal{D}[x] e^{\frac{i}{\hbar}S[x]} \\
\langle x_f, t_f|\, A(\hat{x}(t_1))\, |x_i, t_i\rangle &= \int \mathcal{D}[x] e^{\frac{i}{\hbar}S[x]} A(x(t_1))
\end{aligned}$$

We can also wonder what happens if we plug in two functions in the path integral. Let $t_f > t_2 > t_1 > t_i$, and consider two functions $\mathcal{O}_1(x)$ and $\mathcal{O}_2(x)$. Then,

$$\begin{aligned}
&\int \mathcal{D}[x] e^{\frac{i}{\hbar}S[x]} \mathcal{O}_1(x(t_1)) \mathcal{O}_2(x(t_2)) \\
&\qquad = \int \mathrm{d}x_1 \mathrm{d}x_2 \int \mathcal{D}[x_a]\mathcal{D}[x_b]\mathcal{D}[x_c]\; e^{\frac{i}{\hbar}(S_a+S_b+S_c)} \mathcal{O}_1(x(t_1)) \mathcal{O}_2(x(t_2)) \\
&\qquad = \int \mathrm{d}x_1 \mathrm{d}x_2\, \langle x_f, t_f | x_2, t_2\rangle\, \mathcal{O}_2(x(t_2))\, \langle x_2, t_2 | x_1, t_1\rangle\, \mathcal{O}_1(x(t_1))\, \langle x_1, t_1 | x_i, t_i\rangle \\
&\qquad = \langle x_f, t_f|\, \mathcal{O}_2(\hat{x}(t_2)) \mathcal{O}_1(\hat{x}(t_1))\, |x_i, t_i\rangle\,. \qquad (1.111)
\end{aligned}$$

Notice that on the path integral side (on the left), the functions $\mathcal{O}_1$ and $\mathcal{O}_2$ commute, since they are just numbers. However, on the right side, they do not commute anymore since they contain the **Heisenberg-picture** operators $\hat{x}(t_1)$ and $\hat{x}(t_2)$. In the Schrödinger picture, $\hat{x}$ obviously commutes with itself, but in the Heisenberg picture, $\hat{x}(t)$ involves the hamiltonian and therefore $[\hat{x}(t_1), \hat{x}(t_2)] \neq 0$ in general. In fact, the non-commutativity of the $\mathcal{O}$'s on the right side comes from the assumption that $t_2 > t_1$. If we had assumed $t_1 > t_2$, the order of the $\mathcal{O}$'s would be reversed (see the exercise below).

Exercise 1.6 (Introduction to time-ordering)**.**
In equation (1.111), it was assumed that $t_1 < t_2$. Verify that in the other case, $t_1 > t_2$, one has

$$\int \mathcal{D}[x] e^{\frac{i}{\hbar}S[x]} \mathcal{O}_1(x(t_1)) \mathcal{O}_2(x(t_2)) = \langle x_f, t_f|\, \mathcal{O}_1(\hat{x}(t_1)) \mathcal{O}_2(\hat{x}(t_2))\, |x_i, t_i\rangle\,. \qquad (1.112)$$

Define the **time-ordered product** of two operators as

$$T[\hat{\mathcal{O}}_1(t_1)\hat{\mathcal{O}}_2(t_2)] = \hat{\mathcal{O}}_2(t_2)\hat{\mathcal{O}}_1(t_1)\theta(t_2-t_1) + \hat{\mathcal{O}}_1(t_1)\hat{\mathcal{O}}_2(t_2)\theta(t_1-t_2), \tag{1.113}$$

where we write $\hat{\mathcal{O}}(t) \equiv \mathcal{O}(\hat{x}(t))$ as a shorthand. The generalization to an arbitrary number of $\mathcal{O}$'s is obvious:

$$\boxed{\int \mathcal{D}[x] e^{\frac{i}{\hbar}S[x]} \mathcal{O}_1(x(t_1)) \dots \mathcal{O}_n(x(t_n)) = \langle x_f, t_f | \, T\left[\hat{\mathcal{O}}_1(t_1) \dots \hat{\mathcal{O}}_n(t_n)\right] | x_i, t_i \rangle} \tag{1.114}$$

Question: how could we compute **out of time-order** correlators with path integrals? This will be discussed in lecture 5.

Introduction to the classical limit and useful properties of $S_{\mathbf{cl}}$

Consider the propagator

$$K(x_f, t_f; x_i, t_i) = \int \mathcal{D}[x] e^{\frac{i}{\hbar}S[x]}. \tag{1.115}$$

The classical limit is the limit where $\hbar \to 0$. [8] In this case, we can do a saddle point approximation (see exercise 10 for more details) and write

$$K(x_f, t_f; x_i, t_i) = \int \mathcal{D}[x] e^{\frac{i}{\hbar}S[x]} = e^{\frac{i}{\hbar}S[x_{\rm cl}]} F(x_f, t_f; x_i, t_i), \tag{1.116}$$

where F is some function depending on the boundary conditions. Then, we have

$$-i\hbar\partial_{x_f} K = \left[\partial_{x_f} S_{\rm cl} K + \mathcal{O}(\hbar)\right] K = \left[p_f^{\rm cl} + \mathcal{O}(\hbar)\right] K \tag{1.117}$$

$$i\hbar\partial_{t_f} K = \left[-\partial_{t_f} S_{\rm cl} K + \mathcal{O}(\hbar)\right] K = \left[E_{\rm cl} + \mathcal{O}(\hbar)\right] K. \tag{1.118}$$

Here we used the fact that F does not depend exponentially on $\hbar$ when $\hbar \to 0$. The equalities between derivatives of $S_{\rm cl}$ and the classical momentum and energy are exact relations coming from classical mechanics, and are justified below. It is interesting to see that the **quantum** version of the final momenta and the energy acting on the propagator (the left-hand side) are equal to the **classical** version, plus some correction of order $\hbar$ (the right-hand side).

In order to prove the equalities $\partial_{x_f} S_{\rm cl} = p_f^{\rm cl}$ and $\partial_{t_f} S_{\rm cl} = -E_{\rm cl}$, consider the following definitions:

$$S_{\rm cl} = \int_{t_i}^{t_f} {\rm d}t \; \mathcal{L}[x_c, \dot{x}_c], \quad \text{with} \quad \left[\frac{\rm d}{{\rm d}t}\frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x}\right]_{x=x_c} = 0, \quad \text{and} \quad \begin{cases} x_c(t_i) = x_i \\ x_c(t_f) = x_f \end{cases} \tag{1.119}$$

[8] Note that it would be more precise to say that the action is much bigger than $\hbar$, since it does not make sense to send a dimensionful quantity to 0.

Define now the function f as

$$x_c(t) = f(x_f, t_f, x_i, t_i, t). \tag{1.120}$$

In a way, we are saying that the classical solution obviously depends on which boundary conditions we choose, and the function f reflects this choice explicitly, rather than just writing $x_c(t)$ where the boundary conditions are implicit. We therefore have

$$f(x_f, t_f, x_i, t_i, t = t_i) = x_i, \quad f(x_f, t_f, x_i, t_i, t = t_f) = x_f \tag{1.121}$$

Now we can differentiate either of the expressions in (1.121) with respect to any variable. For example, differentiating the first expression with respect to t_i, we get

$$\left[\frac{\partial}{\partial t_i} x_c + \dot{x}_c\right]_{t=t_i} = 0 \tag{1.122}$$

If we differentiate with respect to t_f or x_i, we simply get

$$\left[\frac{\partial}{\partial t_f} x_c\right]_{t=t_i} = 0 \tag{1.123}$$

$$\left[\frac{\partial}{\partial x_i} x_c\right]_{t=t_i} = 1 \tag{1.124}$$

The same ideas can be applied to the other expression in equation (1.121):

$$\left[\frac{\partial}{\partial t_i} x_c\right]_{t=t_f} = 0 \tag{1.125}$$

$$\left[\frac{\partial}{\partial t_f} x_c + \dot{x}_c\right]_{t=t_f} = 0 \tag{1.126}$$

$$\left[\frac{\partial}{\partial x_f} x_c\right]_{t=t_f} = 1 \tag{1.127}$$

$$\dots$$

These identities are useful because they allow us to compute derivatives of the classical action. Indeed,

$$\partial_{t_f} S_{\text{cl}} = \partial_{t_f} \int_{t_i}^{t_f} \mathrm{d}t \; \mathcal{L}[x_c, \dot{x}_c] \tag{1.128}$$

$$= \mathcal{L}[x_c, \dot{x}_c]_{t=t_f} + \int_{t_i}^{t_f} \mathrm{d}t \; \left.\frac{\partial \mathcal{L}}{\partial x}\right|_{x_c} \partial_{t_f} x_c + \left.\frac{\partial \mathcal{L}}{\partial \dot{x}}\right|_{x_c} \partial_{t_f} \dot{x}_c \tag{1.129}$$

$$= \mathcal{L}[x_c, \dot{x}_c]_{t=t_f} + \left[\left.\frac{\partial \mathcal{L}}{\partial \dot{x}}\right|_{x_c} \partial_{t_f} x_c\right]_{t_i}^{t_f} - \int_{t_i}^{t_f} \mathrm{d}t \; \underbrace{\left[\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x}\right]_{x=x_c}}_{=0 \text{ (E.O.M.)}} \partial_{t_f} x_c, \tag{1.130}$$

where in the last line we integrated by parts. Using equations (1.123) and (1.126), we find

$$\partial_{t_f} S_{\rm cl} = \left[\mathcal{L}[x_c, \dot{x}_c] - \left.\frac{\partial \mathcal{L}}{\partial \dot{x}}\right|_{x_c} \dot{x}_c \right]_{t=t_f} = -\left[p_c \dot{x}_c - \mathcal{L}[x_c, \dot{x}_c] \right]_{t=t_f} \tag{1.131}$$

$$= -\left. H \right|_{t=t_f} = -E_{\rm cl} \tag{1.132}$$

Similarly, we have

$$\partial_{x_f} S_{\rm cl} = \int_{t_i}^{t_f} \mathrm{d}t \ \left.\frac{\partial \mathcal{L}}{\partial x}\right|_{x_c} \partial_{x_f} x_c + \left.\frac{\partial \mathcal{L}}{\partial \dot{x}}\right|_{x_c} \partial_{x_f} \dot{x}_c \tag{1.133}$$

$$= \left[\left.\frac{\partial \mathcal{L}}{\partial \dot{x}}\right|_{x_c} \partial_{x_f} x_c \right]_{t_i}^{t_f} + \int_{t_i}^{t_f} \mathrm{d}t \ \left[\left.\frac{\partial \mathcal{L}}{\partial x}\right|_{x_c} - \frac{\mathrm{d}}{\mathrm{d}t} \left.\frac{\partial \mathcal{L}}{\partial \dot{x}}\right|_{x_c} \right] \partial_{x_f} x_c \tag{1.134}$$

$$= p_f^{\rm cl}, \tag{1.135}$$

where in the last line we used (1.127).

Summary of Lecture 3

- Gelfand-Yaglom formula:

$$K(x_f, t_f; x_i, t_i) = e^{\frac{i}{\hbar} S[x_c]} \sqrt{\frac{m}{2\pi i \hbar \, \varphi(t_f)}}, \quad \text{where } \ddot{\varphi}(t) = -\omega^2(t)\varphi(t), \ \begin{cases} \varphi(t_i) = 0 \\ \dot{\varphi}(t_i) = 1 \end{cases}$$

- Operator matrix elements:

$$\int \mathcal{D}[x] e^{\frac{i}{\hbar} S[x]} \mathcal{O}_1(x(t_1)) \dots \mathcal{O}_n(x(t_n)) = \langle x_f, t_f | \, T \left[\hat{\mathcal{O}}_1(t_1) \dots \hat{\mathcal{O}}_n(t_n) \right] | x_i, t_i \rangle$$

- Properties of the classical action:

$$\partial_{x_f} S_{\rm cl} = p_f^{\rm cl}, \quad \partial_{t_f} S_{\rm cl} = -E_{\rm cl}$$

Lecture 4 - Quantum Mechanics in Your Face.

In this special lecture we discuss a famous lecture by Sidney Coleman:
`https://arxiv.org/abs/2011.12671`
`https://www.youtube.com/watch?v=EtyNMlXN-sw`

Chapter 2

Functional and Euclidean methods

Lecture 5 - Euclidean path integral

Euclidean path integrals are the most useful in practice because of their convergence properties. They are very common in Quantum Field Theory (QFT) and Statistical Mechanics, and are used to perform perturbation theory through the use of **Feynman diagrams**. They will also be useful to compute out of time-order correlators, which we mentioned in Lecture 3.

Define the **Euclidean propagator** K_E as

$$K_E(x_f, x_i, \beta) = \langle x_f | \, e^{-\frac{\beta}{\hbar}\hat{H}} \, |x_i\rangle \,, \quad \beta \geq 0 \ ^{1} \tag{2.2}$$

Note that it is possible to go from the usual propagator $K(x_f, T, x_i, 0)$ to the Euclidean propagator by **analytic continuation**, through the replacement $T \to -i\beta$. For this reason, this is sometimes called "evolution in imaginary time". This replacement is where the name **Euclidean** comes from. Indeed, the metric of Minkowski spacetime is

$$\mathrm{d}s_M^2 = -\mathrm{d}t^2 + \mathrm{d}\mathbf{x}^2$$

Now if we set $t \to -i\tau$, we get the Euclidean metric:

$$\mathrm{d}s_E^2 = \mathrm{d}\tau^2 + \mathrm{d}\mathbf{x}^2,$$

which is just Cartesian space with one extra coordinate. Notice that Lorentz transformations, which leave Minkowski spacetime invariant, become simply 4D rotations, which leave Euclidean space invariant.

[1] More generally $\mathrm{Re}(\beta) > 0$. The reason for this is that $\hat{H}$ is not bounded from above. More explicitly,

$$\langle x_f | \, e^{-\frac{\beta}{\hbar}\hat{H}} \, |x_i\rangle = \sum_E \langle x_f | E\rangle \, \langle E | x_i\rangle \, e^{-\frac{\beta}{\hbar}E}, \tag{2.2}$$

which diverges when $\mathrm{Re}(\beta) < 0$ since there is an infinite number of states with increasing energy.

Path integral representation of K_E

We go through the same steps we did to build the path integral representation of the Minkowski propagator. Let $x_0 = x_i$, $x_N = x_f$, and $\beta = N\epsilon$. Then,

$$K_E(x_f, x_i, \beta) = \langle x_N | \, e^{-\frac{\epsilon}{\hbar}\hat{H}} \int \mathrm{d}x_{N-1} \, |x_{N-1}\rangle \langle x_{N-1}| \ldots \int \mathrm{d}x_1 \, |x_1\rangle \langle x_1| \, e^{-\frac{\epsilon}{\hbar}\hat{H}} \, |x_0\rangle \quad (2.3)$$

$$= \int \mathrm{d}x_{N-1} \ldots \mathrm{d}x_1 \, \prod_{i=1}^{N} \langle x_i| \, e^{-\frac{\epsilon}{\hbar}\hat{H}} \, |x_{i-1}\rangle \, . \quad (2.4)$$

Consider now

$$\left\langle x' \right| e^{-\frac{\epsilon}{\hbar}\hat{H}} \left| x \right\rangle = \int \mathrm{d}p \, \left\langle x' | p \right\rangle \langle p | x \rangle \, e^{-\frac{\epsilon}{\hbar}\left(\frac{p^2}{2m} + V(x)\right)} \quad (2.5)$$

$$= \int \frac{\mathrm{d}p}{2\pi\hbar} \, e^{\frac{i}{\hbar}p(x'-x)} e^{-\frac{\epsilon}{\hbar}\left(\frac{p^2}{2m} + V(x)\right)}. \quad (2.6)$$

Now after doing the Gaussian integral, we find

$$\left\langle x' \right| e^{-\frac{\epsilon}{\hbar}\hat{H}} \left| x \right\rangle = \sqrt{\frac{m}{2\pi\hbar\epsilon}} e^{-\frac{1}{\hbar}\left(\frac{1}{2}m\left(\frac{x'-x}{\epsilon}\right)^2 + V(x)\right)\epsilon}, \quad (2.7)$$

and therefore

$$K_E(x_f, x_i, \beta) = \frac{1}{A_E} \int \prod_{k=1}^{N-1} \frac{\mathrm{d}x_k}{A_E} \, e^{-\frac{1}{\hbar}\sum_{i=1}^{N}\left(\frac{1}{2}m\dot{x}_i^2 + V(x)\right)\epsilon} \quad \left(\frac{1}{A_E} \equiv \frac{m}{2\pi\hbar\epsilon}\right). \quad (2.8)$$

Taking the limit $\epsilon \to 0$, we find

$$K_E(x_f, x_i, \beta) = \lim_{\epsilon\to 0} \frac{1}{A_E} \int \prod_{k=1}^{N-1} \frac{\mathrm{d}x_k}{A_E} \, e^{-\frac{1}{\hbar}\int_0^\beta \mathrm{d}\tau \, \left(\frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + V(x)\right)} \quad (2.9)$$

$$\equiv \int \mathcal{D}_E[x] \, e^{-\frac{S_E[x]}{\hbar}}, \quad \text{where } S_E[x] = \int_0^\beta \mathrm{d}\tau \left[\frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + V(x)\right]$$

Notice the two main differences compared to the Minkowski path integral: there is no i in the exponent, and the action now has a $+V(x)$ instead of a $-V(x)$.

Notice that this result could have also been attained through analytic continuation. Indeed, we have

$$\left.\begin{array}{r} t \to -i\tau \\ T \to -i\beta \end{array}\right\} \implies \mathrm{d}t \to -i\mathrm{d}\tau, \quad \left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 \to -\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2, \quad (2.10)$$

and therefore

$$iS[x] = i\int_0^T \mathrm{d}t \, \left[\frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x)\right] \to \int_0^\beta \mathrm{d}\tau \, \left[-\frac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 - V(x)\right] = -S_E[x].$$

The path integral measures of the Minkowski P.I. and the Euclidean P.I. are also related through analytic continuation.

The Euclidean path integral

$$\int \mathcal{D}_E[x] e^{-\frac{1}{\hbar}S_E}$$

is dominated by paths with minimal S_E. The other paths are exponentially suppressed. Notice that if $V(x)$ is bounded from below (which is usually the case), then so is $S_E[x]$. This is why the Euclidean path integral has better convergence properties than the Minkowski version, where each path is weighted with a pure phase $e^{iS/\hbar}$.

Remark:
A link between the Euclidean path integral and statistical mechanics can be drawn by interpreting the exponential in the path integral as a Boltzmann weight:

$$e^{-\frac{1}{\hbar}S_E} \sim e^{-\frac{E}{k_B T}}. \tag{2.11}$$

One can then perform numerical Monte-Carlo simulations, where we sum over random paths with probability distribution given by $e^{-S_E/\hbar}$. Even if the Minkowski path integral for a system cannot be computed exactly, one can use numerical methods to solve the Euclidean path integral[2].

Connection with statistical mechanics

Let $|n\rangle$ be the energy eigenstates. Then,

$$K_E(x_f, x_i, \beta) = \langle x_f | \, e^{-\frac{\beta}{\hbar}\hat{H}} \left(\sum_n |n\rangle \langle n| \right) |x_i\rangle \tag{2.12}$$

$$= \sum_n \psi_n(x_f)\psi_n^*(x_i) e^{-\frac{\beta}{\hbar}E_n} \tag{2.13}$$

$$\implies \int \mathrm{d}x \, K_E(x, x, \beta) = \sum_n \underbrace{\int \mathrm{d}x |\psi_n(x)|}_{=1} e^{-\frac{\beta}{\hbar}E_n}. \tag{2.14}$$

The right-hand side of the last line is exactly the **thermal partition function** Z from statistical mechanics, evaluated at temperature $T = \frac{\hbar}{k_B \beta}$ (here by T we denote the temperature, not the period):

$$\boxed{\int \mathrm{d}x \, K_E(x, x, \beta) = \sum_n e^{-\frac{\beta}{\hbar}E_n} = Z\left(T = \frac{\hbar}{k_B \beta}\right)} \tag{2.15}$$

[2] An example where this is used is non-abelian gauge theories, which model the strong nuclear interaction. Many observables cannot be computed in the Minkowski path integral, but can be solved numerically by going to the Euclidean regime and discretizing spacetime (Lattice Gauge Theory).

For clarity, we will denote $Z(T = \frac{\hbar}{k_B \beta}) \equiv Z(\beta)$.

Our formalism allows us to have a path integral representation of the partition function:

$$\boxed{Z(\beta) = \int \mathrm{d}y \int_{\substack{x(0)=y \\ x(\beta)=y}} \mathcal{D}_E[x] e^{-\frac{S_E[x]}{\hbar}} \equiv \int_{x(0)=x(\beta)} \mathcal{D}_E[x] e^{-\frac{S_E[x]}{\hbar}}} \tag{2.16}$$

The sum is over **periodic paths**, with period β in imaginary time.

Note that we can also write the partition function as a trace, since

$$Z(\beta) = \int \mathrm{d}x K_E(x, x, \beta) = \int \mathrm{d}x \, \langle x | \, e^{-\frac{\beta}{\hbar}\hat{H}} \, | x \rangle = \mathrm{Tr}\left(e^{-\frac{\beta}{\hbar}\hat{H}}\right)$$

Example: Harmonic Oscillator
In this example we derive the Euclidean propagator for the HO by analytic continuation of the Minkowski propagator. Recall that

$$K^{(\mathrm{HO})}(x_f, T; x_i, 0) = e^{-i\frac{\pi}{2}\,\mathrm{int}\left(\frac{\omega T}{\pi}\right)} \sqrt{\frac{m\omega}{2\pi i\hbar |\sin(\omega T)|}} e^{i\frac{m\omega}{2\hbar}\frac{\left(x_f^2 + x_i^2\right)\cos(\omega T) - 2x_i x_f}{\sin(\omega T)}}.$$

In this example we assume that T is small enough that we can neglect the phase term, and write $\sin(\omega T) > 0$. In that case,

$$K^{(\mathrm{HO})}(x_f, T; x_i, 0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}} e^{i\frac{m\omega}{2\hbar}\frac{\left(x_f^2 + x_i^2\right)\cos(\omega T) - 2x_i x_f}{\sin(\omega T)}}.$$

To get the Euclidean propagator, let $T \to -i\beta$. Then,

$$\boxed{K_E^{(\mathrm{HO})}(x_f, x_i, \beta) = \sqrt{\frac{m\omega}{2\pi\hbar \sinh(\omega\beta)}} e^{-\frac{m\omega}{2\hbar}\frac{\left(x_f^2 + x_i^2\right)\cosh(\omega\beta) - 2x_i x_f}{\sinh(\omega\beta)}}} \tag{2.17}$$

It is also possible to derive this result directly from the path integral representation of K_E.

Exercise 2.1 (HO energy levels from the Euclidean propagator)**.**
Using the explicit form for the Euclidean propagator of the harmonic oscillator (eq. 2.17) and its relation to the partition function (eq. 2.15), compute the energy levels of the harmonic oscillator.

From the exercise above, one can see that the Euclidean propagator can be used to derive the energy spectrum. In fact, the propagator also "knows" the eigenfunctions of the system - see equation (2.13).

Euclidean n-point correlators

Consider now a Euclidean time interval $[-\beta/2, \beta/2]$, with $\beta > 0$, and let $\tau_i \in [-\beta/2, \beta/2]$, $i = 1, \ldots, n$. Consider then the following path integral:

$$\int_{x(-\beta/2)=x_i}^{x(\beta/2)=x_f} \mathcal{D}[x]_E \, e^{-\frac{S_E[x]}{\hbar}} x(\tau_1) \ldots x(\tau_n). \tag{2.18}$$

By analogy with the Minkowski case that we computed in lecture 3, we find that this path integral is equal to the time-ordered correlator

$$\langle x_f | \, e^{-\frac{\beta \hat{H}}{2\hbar}} \, T[\hat{x}_E(\tau_1) \ldots \hat{x}_E(\tau_n)] \, e^{-\frac{\beta \hat{H}}{2\hbar}} \, |x_i\rangle \,, \tag{2.19}$$

where

$$\hat{x}_E(\tau) \equiv e^{\frac{\tau}{\hbar}\hat{H}} \hat{x}_E e^{-\frac{\tau}{\hbar}\hat{H}} = \hat{x}(-i\tau). \tag{2.20}$$

$\hat{x}_E(\tau)$ is the analytic continuation of the Heisenberg picture position operator.

We now attempt to find an expression in terms of path integral of another object: the **vacuum expectation value** of the time-ordered product

$$\langle 0 | \, T[\hat{x}_E(\tau_1) \ldots \hat{x}_E(\tau_n)] \, |0\rangle \,, \tag{2.21}$$

where $|0\rangle$ is the vacuum (the ground state of the system). To do so, we could look at the limit $\beta \to \infty$, since it corresponds to the temperature going to 0. At zero temperature, we only get the contribution from the ground state, and we therefore hope to find the expression above. Indeed, we have

$$\begin{aligned} &\lim_{\beta\to\infty} \langle x_f | \, e^{-\frac{\beta \hat{H}}{2\hbar}} \, T[\hat{x}_E(\tau_1) \ldots \hat{x}_E(\tau_n)] \, e^{-\frac{\beta \hat{H}}{2\hbar}} \, |x_i\rangle \\ &\qquad = \sum_{n,m} \lim_{\beta\to\infty} e^{-\frac{\beta(E_n+E_m)}{2\hbar}} \, \langle x_f|n\rangle \, \langle n| \, T[\hat{x}_E(\tau_1) \ldots \hat{x}_E(\tau_n)] \, |m\rangle \, \langle m|x_i\rangle \,. \end{aligned}$$

Now, assuming that the energy levels are positive, we see that every term is exponentially suppressed. The leading order term among all these is the one with the smallest energy, i.e. the one with $n = m = 0$. We therefore find

$$\begin{aligned} &\lim_{\beta\to\infty} \langle x_f | \, e^{-\frac{\beta \hat{H}}{2\hbar}} \, T[\hat{x}_E(\tau_1) \ldots \hat{x}_E(\tau_n)] \, e^{-\frac{\beta \hat{H}}{2\hbar}} \, |x_i\rangle \\ &\qquad = e^{-\frac{\beta E_0}{\hbar}} \psi_0(x_f) \psi_0^*(x_i) \, \langle 0 | \, T[\hat{x}_E(\tau_1) \ldots \hat{x}_E(\tau_n)] \, |0\rangle \left(1 + \mathcal{O}\left(e^{-\frac{\beta(E_1-E_0)}{2\hbar}}\right)\right) \end{aligned}$$

We can see the vacuum expectation value we were looking for. However, there are extra factors in front which we want to get rid of. Note that

$$\begin{aligned} \lim_{\beta\to\infty} \langle x_f | \, e^{-\frac{\beta}{\hbar}\hat{H}} \, |x_i\rangle &= \sum_n \lim_{\beta\to\infty} e^{-\frac{\beta}{\hbar}E_n} \psi_n(x_f) \psi_n^*(x_i) \\ &= e^{-\frac{\beta E_0}{\hbar}} \psi_0(x_f) \psi_0^*(x_i) \left(1 + \mathcal{O}\left(e^{-\frac{\beta(E_1-E_0)}{\hbar}}\right)\right), \end{aligned}$$

which cancels exactly the pieces we did not want! We can therefore write

$$\langle 0|\, T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\,|0\rangle = \lim_{\beta\to\infty} \frac{\langle x_f|\, e^{-\frac{\beta\hat{H}}{2\hbar}}\, T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\, e^{-\frac{\beta\hat{H}}{2\hbar}}\,|x_i\rangle}{\langle x_f|\, e^{-\frac{\beta}{\hbar}\hat{H}}\,|x_i\rangle} \tag{2.22}$$

$$= \lim_{\beta\to\infty} \frac{\int \mathcal{D}[x]_E\, e^{-\frac{S_E[x]}{\hbar}} x(\tau_1)\dots x(\tau_n)}{\int \mathcal{D}[x]_E\, e^{-\frac{S_E[x]}{\hbar}}}, \tag{2.23}$$

where the path integrals' boundary conditions are $x(-\beta/2) = x_i$, $x(\beta/2) = x_f$. [3]

Remark:
Note that on the left-hand side, there is no dependency on x_i or x_f, which tells us that the boundary conditions do not matter in the limit $\beta \to \infty$. In other words, if we choose $x(-\beta/2) = x_i'$ and $x(\beta/2) = x_f'$ and compute the path integrals with these boundary conditions, the resulting vacuum expectation value on the left will not be changed.

It is convenient to define the **Dirichlet n-point function** G_D as

$$\hbar^{n/2} G_D(\tau_1,\dots,\tau_n) \equiv \frac{\langle x_f = 0|\, e^{-\frac{\beta\hat{H}}{2\hbar}}\, T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\, e^{-\frac{\beta\hat{H}}{2\hbar}}\,|x_i = 0\rangle}{\langle x_f = 0|\, e^{-\frac{\beta}{\hbar}\hat{H}}\,|x_i = 0\rangle} \tag{2.24}$$

$$= \frac{\int \mathcal{D}[x]_E\, e^{-\frac{S_E[x]}{\hbar}} x(\tau_1)\dots x(\tau_n)}{\int \mathcal{D}[x]_E\, e^{-\frac{S_E[x]}{\hbar}}}, \tag{2.25}$$

where the factor $\hbar^{n/2}$ is for later convenience. Note that we removed the limits $\beta \to \infty$, and that we set the boundary conditions to be **Dirichlet B.C.**: $x_i = x_f = 0$. Furthermore, do not confuse the position eigenstate $|x = 0\rangle$ and the ground state $|0\rangle$. We find back the vacuum expectation value by taking the limit $\beta \to \infty$, since the boundary conditions do not matter in that limit.

$$\langle 0|\, T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\,|0\rangle = \lim_{\beta\to\infty} \hbar^{n/2} G_D(\tau_1,\dots,\tau_n) \tag{2.26}$$

Thermal n-point functions

Recall that

$$Z(\beta) = \int_{x(0)=x(\beta)} \mathcal{D}_E[x] e^{-\frac{S_E[x]}{\hbar}} = \mathrm{Tr}\Big(e^{-\frac{\beta}{\hbar}\hat{H}}\Big) \tag{2.27}$$

We can now compute the **thermal average** of the time-ordered products of $\hat{x}_E(\tau)$:

$$\langle T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\rangle_\beta = \frac{1}{Z(\beta)}\,\mathrm{Tr}\left(e^{-\frac{\beta}{\hbar}\hat{H}} T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\right) \tag{2.28}$$

[3] Here we assumed that $\psi_0(x_f)\psi_0^*(x_i) \neq 0$.

This again has a path integral representation, where now we have **periodic boundary conditions**:

$$\langle T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\rangle_\beta = \frac{\int_{x(-\beta/2)=x(\beta/2)}\mathcal{D}[x]_E\, e^{-\frac{S_E[x]}{\hbar}} x(\tau_1)\dots x(\tau_n)}{\int_{x(-\beta/2)=x(\beta/2)}\mathcal{D}[x]_E\, e^{-\frac{S_E[x]}{\hbar}}} \tag{2.29}$$

As before, we define the **Periodic n-point function** G_P as

$$\hbar^{n/2}G_P(\tau_1,\dots,\tau_n) \equiv \langle T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\rangle_\beta \tag{2.30}$$

$$= \frac{\int_{x(-\beta/2)=x(\beta/2)}\mathcal{D}[x]_E\, e^{-\frac{S_E[x]}{\hbar}} x(\tau_1)\dots x(\tau_n)}{\int_{x(-\beta/2)=x(\beta/2)}\mathcal{D}[x]_E\, e^{-\frac{S_E[x]}{\hbar}}}. \tag{2.31}$$

Exercise 2.2 (Ground state projector)**.** *Show that*

$$\lim_{\beta\to\infty}\frac{1}{Z(\beta)}e^{-\frac{\beta}{\hbar}\hat{H}} = |0\rangle\langle 0| \tag{2.32}$$

Hint: compute matrix elements of the operators above in the energy basis.

Now as before, we would like to take the limit $\beta\to\infty$. Using equation 2.32, we find

$$\lim_{\beta\to\infty}\langle T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\rangle_\beta = \lim_{\beta\to\infty}\frac{1}{Z(\beta)}\operatorname{Tr}\left(e^{-\frac{\beta}{\hbar}\hat{H}}T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\right) \tag{2.33}$$

$$= \langle 0|\, T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\,|0\rangle\,, \tag{2.34}$$

and therefore

$$\boxed{\langle 0|\, T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_n)]\,|0\rangle = \lim_{\beta\to\infty}\hbar^{n/2}G_D(\tau_1,\dots,\tau_n) = \lim_{\beta\to\infty}\hbar^{n/2}G_P(\tau_1,\dots,\tau_n)} \tag{2.35}$$

This explicitly shows that, in the $\beta\to\infty$ limit, the boundary conditions with which we compute the n-point functions does not matter; they both give the VEV of the time-ordered product of $\hat{x}_E$'s. In the next lecture, we will develop tools to compute the functions G_D and G_P perturbatively.

From Euclidean to real time

For ease of notation, we now give a name to the vacuum expectation value of the time-ordered product:

$$G_E(\tau_1,\dots,\tau_N) = \langle 0|\, T[\hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_N)]\,|0\rangle \tag{2.36}$$

How to obtain a correlation function in real (Lorentzian) time starting from this Euclidean correlation function? One way is to consider the substitution $\tau\to it$, or more precisely the **Wick rotation**

$$\tau = e^{i\theta}t, \quad \theta\in[0,\pi/2], \tag{2.37}$$

where $\theta = 0$ corresponds to Euclidean time and $\theta = \pi/2$ corresponds to real time. Doing this transformation preserves the time-ordering, since if $|\tau_i| > |\tau_j|$, then $t_i > t_j$. The time-ordered VEV in real time is therefore

$$\langle 0| T[\hat{x}(t_1)\dots\hat{x}(t_N)] |0\rangle = G_E(it_1,\dots,it_N). \tag{2.38}$$

The careful reader may wonder if such analytic continuation of G_E is legal. Indeed, it is important to ask what is the domain of analyticity of the Euclidean correlator. Consider ordered τ_i's, such that $\tau_1 > \ldots > \tau_N$.Then

$$\begin{aligned} G_E(\tau_1,\dots,\tau_N) &= \langle 0| \hat{x}_E(\tau_1)\dots\hat{x}_E(\tau_N) |0\rangle & (2.39)\\ &= e^{\frac{1}{\hbar}E_0(\tau_1-\tau_N)} \langle 0| \hat{x}_E e^{-\frac{1}{\hbar}\hat{H}(\tau_1-\tau_2)}\hat{x}_E\dots\hat{x}_E e^{-\frac{1}{\hbar}\hat{H}(\tau_{N-1}-\tau_N)}\hat{x}_E |0\rangle & (2.40)\\ &= e^{\frac{1}{\hbar}E_0(\tau_1-\tau_N)} \sum_{m_1,\dots,m_N} e^{-\frac{1}{\hbar}E_1(\tau_1-\tau_2)}\dots e^{-\frac{1}{\hbar}E_{N-1}(\tau_{N-1}-\tau_N)} \\ &\qquad \cdot \langle 0| \hat{x}_E |m_1\rangle \langle m_1| \hat{x}_E |m_2\rangle \dots \langle m_{N-1}| \hat{x}_E |0\rangle & (2.41) \end{aligned}$$

It is now easy to consider complex τ_i's. We see that in order for the sums to converge, we need $\mathrm{Re}(\tau_k - \tau_{k+1}) > 0$. In the case of a Wick rotation $\tau_k \to e^{i\theta}t_k$, we must have

$$\mathrm{Re}\left(e^{i\theta}(t_k - t_{k+1})\right) = \cos(\theta)(t_k - t_{k+1}) > 0$$

Now since we assumed that the τ's were ordered, so must the t_k's, and since $\theta \in [0, \pi/2[$, the inequality above is respected. Notice that real time is at the boundary of the domain of analyticity.

We can now look at the following limit:

$$\lim_{\substack{\epsilon_k\to 0\\ \epsilon_1>\ldots>\epsilon_N}} G_E(\epsilon_1 + it_1,\dots,\epsilon_N + it_N) \tag{2.42}$$

This is convergent because of the ordering of the ϵ's. Furthermore, this will be equal to the real time VEV, where the ordering is determined by the ordering of the ϵ's, not the t's!

$$\lim_{\substack{\epsilon_k\to 0\\ \epsilon_1>\ldots>\epsilon_N}} G_E(\epsilon_1 + it_1,\dots,\epsilon_N + it_N) = \langle 0| \hat{x}(t_1)\dots\hat{x}(t_N) |0\rangle, \quad \forall\, t_i \in \mathbb{R} \tag{2.43}$$

On the right-hand side, we have the **out of time-order** correlator that we wondered about in lecture 3. Therefore, any ordering in real time can be obtained from this continuation of the Euclidean correlator G_E. This procedure, for the case $N = 2$, is highlighted in more details in exercise 13.

Summary of Lecture 5

- Euclidean path integral:

$$K_E(x_f, x_i; \beta) = \langle x_f | \, e^{-\frac{\beta}{\hbar}\hat{H}} \, | x_i \rangle = \int \mathcal{D}_E[x] e^{-\frac{S_E}{\hbar}},$$

  where S_E can be obtained from S by sending $t \to -i\tau$.

- Thermal partition function:

$$Z(\beta) = \mathrm{Tr}\left(e^{-\frac{\beta}{\hbar}\hat{H}}\right) = \int \mathrm{d}x K_E(x, x; \beta) = \int_{x(0)=x(\beta)} \mathcal{D}_E[x] e^{-\frac{S_E}{\hbar}}$$

- Dirichlet and periodic n-point functions:

$$\hbar^{n/2} G_D(\tau_1, \ldots, \tau_n) = \frac{\int_{x(-\beta/2)=0}^{x(\beta/2)=0} \mathcal{D}[x]_E \, e^{-\frac{S_E[x]}{\hbar}} x(\tau_1) \ldots x(\tau_n)}{\int_{x(-\beta/2)=0}^{x(\beta/2)=0} \mathcal{D}[x]_E \, e^{-\frac{S_E[x]}{\hbar}}}$$

$$\hbar^{n/2} G_P(\tau_1, \ldots, \tau_n) = \frac{\int_{x(-\beta/2)=x(\beta/2)} \mathcal{D}[x]_E \, e^{-\frac{S_E[x]}{\hbar}} x(\tau_1) \ldots x(\tau_n)}{\int_{x(-\beta/2)=x(\beta/2)} \mathcal{D}[x]_E \, e^{-\frac{S_E[x]}{\hbar}}}$$

- Independence of boundary conditions:

$$\left.\begin{array}{l} \lim\limits_{\beta\to\infty} \hbar^{n/2} G_D(\tau_1, \ldots, \tau_n) \\ \lim\limits_{\beta\to\infty} \hbar^{n/2} G_P(\tau_1, \ldots, \tau_n) \end{array}\right\} = \langle 0 | \, T\left[\hat{x}_E(\tau_1) \ldots \hat{x}_E(\tau_n)\right] | 0 \rangle \equiv G_E(\tau_1, \ldots, \tau_n)$$

- Wick rotation:

$$\tau_j = e^{i\theta} t_j, \quad \theta \in [0, \pi/2]. \qquad \begin{cases} \theta = 0 : \text{ Euclidean} \\ \theta = \pi/2 : \text{ Minkowski} \end{cases}$$

$$G_E(\tau_1 = e^{i\theta} t_1, \ldots, \tau_n = e^{i\theta} t_n) \xrightarrow[\theta\to\pi/2]{} \langle 0 | \, T\left[\hat{x}(t_1) \ldots \hat{x}(t_n)\right] | 0 \rangle$$

- Out of time order correlator:

$$\langle 0 | \, \hat{x}(t_1) \ldots \hat{x}(t_N) \, | 0 \rangle = \lim_{\substack{\epsilon_k \to 0 \\ \epsilon_1 > \ldots > \epsilon_N}} G_E(\epsilon_1 + i t_1, \ldots, \epsilon_N + i t_N)$$

Lecture 6 - Functional methods

The main idea of functional methods is to couple the system to an external **source** in order to probe the system. This idea is useful both in experimental and in theoretical physics.

Examples:

- Magnetic field on a spin system
- Curved geometry in QFT
- EM waves on a system with charged particles

In practice:
We work in the Euclidean regime from now on. Define $Z[\beta, J]$ as the partition function of the system coupled to an external source $J(\tau)$:

$$Z[\beta, J] \equiv \int_{x(-\beta/2)=x(\beta/2)} \mathcal{D}_E[x] \exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \, [\mathcal{L}_E - x(\tau)J(\tau)]\right) \tag{2.44}$$

This is useful because we can make the periodic n-point function G_P appear by taking derivatives with respect to J. Indeed, each derivative will bring down a factor of $x(\tau)$. Explicitly,

$$\hbar^n \frac{\delta}{\delta J(\tau_1)} \dots \frac{\delta}{\delta J(\tau_n)} Z[\beta, J] = \int \mathcal{D}_E[x] \, x(\tau_1) \dots x(\tau_n) e^{-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \, [\mathcal{L}_E - x(\tau)J(\tau)]} \tag{2.45}$$

Now that we have the appropriate factors of $x(\tau)$, we can set $J = 0$ to recover G_P:

$$\boxed{\hbar^{n/2} G_P(\tau_1, \dots, \tau_n) = \frac{\hbar^n}{Z[\beta, 0]} \frac{\delta}{\delta J(\tau_1)} \dots \frac{\delta}{\delta J(\tau_n)} Z[\beta, J]\Big|_{J=0}} \tag{2.46}$$

We can do the same exact process with Dirichlet (instead of periodic) boundary conditions:

$$K_E[\beta, J] \equiv \int_{x(-\beta/2)=0}^{x(\beta/2)=0} \mathcal{D}_E[x] \exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \, [\mathcal{L}_E - x(\tau)J(\tau)]\right) \tag{2.47}$$

$$\implies \boxed{\hbar^{n/2} G_D(\tau_1, \dots, \tau_n) = \frac{\hbar^n}{K_E[\beta, 0]} \frac{\delta}{\delta J(\tau_1)} \dots \frac{\delta}{\delta J(\tau_n)} K_E[\beta, J]\Big|_{J=0}} \tag{2.48}$$

We see that the n-point functions G_P and G_D are encoded into (derivatives of) the partition function / propagator **with the added source** J. Before going on to study general complicated systems with an external source, it is helpful to consider the usual gaussian problem in the presence of J: the forced harmonic oscillator.

The forced harmonic oscillator

Consider

$$K_E[\beta, J] = \int_{x(-\beta/2)=0}^{x(\beta/2)=0} \mathcal{D}_E[x] \exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \left[\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + \frac{m}{2}\omega^2 x^2 - x(\tau)J(\tau)\right]\right)$$

Note that we can express the Euclidean action in the following way:

$$S_E = \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \left[\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 + \frac{m}{2}\omega^2 x^2\right] \tag{2.49}$$

$$= \frac{1}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, x(\tau)\left[-m\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + m\omega^2\right] x(\tau) \tag{2.50}$$

$$= \frac{1}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2\, x(\tau_1) O(\tau_1, \tau_2) x(\tau_2), \tag{2.51}$$

where

$$O(\tau_1, \tau_2) \equiv m\left[-\frac{\partial^2}{\partial\tau_1^2} + \omega^2\right]\delta(\tau_1 - \tau_2). \tag{2.52}$$

This is a "nice" form because it looks like the Gaussian integrals in n dimensions we studied in Lecture 2. The operator $O(\tau_1, \tau_2)$ contains a derivative acting on a delta function, which can be dealt with by using integration by parts (more details are given in B.2). We can now express the integral in the exponential of K_E by completing the square. We present here the conceptual reasoning, while the more rigorous version is done in the exercises[4].

The exponential in the propagator is essentially of the form

$$I = -\frac{1}{2}x^T O x + J^T x \tag{2.53}$$

if we think of O as a big matrix and x, J as vectors. We would like to get rid of the linear piece to be able to integrate using the usual Gaussian integration techniques. We can introduce some new vector a:

$$I = -\frac{1}{2}(x^T + a^T)O(x + a) + \frac{1}{2}(a^T O + J^T)x + \frac{1}{2}x^T(Oa + J) + \frac{1}{2}a^T O a \tag{2.54}$$

At this point, we set $Oa + J = 0$, or $a = -O^{-1}J$. Then, as long as O is symmetric, we get

$$I = -\frac{1}{2}y^T O y + \frac{1}{2}J^T O^{-1} J \quad (y = x - O^{-1}J) \tag{2.55}$$

[4]Exercise (12) is done in Lorentzian signature and (14) in Euclidean signature. Note that they do not immediately consider Dirichlet boundary conditions, but first perform a shift $x = x_c + y$, which leads to Dirichlet BC ($y = 0$ at the endpoints).

In this form, the exponential splits into a Gaussian piece which will just become $K_E[\beta, 0]$ after a change of variable in the path integral ($\mathcal{D}_E[x] \to \mathcal{D}_E[y]$), and another piece which is **independent of** y. This other piece can just be brought out in front of the path integral, and we therefore expect

$$K_E[\beta, J] = K_E[\beta, 0] \cdot \exp\left(\frac{1}{2\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2\, J(\tau_1) O^{-1}(\tau_1, \tau_2) J(\tau_2)\right), \tag{2.56}$$

where now instead of using finite dimensional matrices for O and J, we went back to the infinite dimensional case. The inverse of the operator $O(\tau_1, \tau_2)$ will be given by its Green's function $G(\tau_1, \tau_2)$ (with appropriate boundary conditions). $G(\tau_1, \tau_2)$ satisfies

$$\underbrace{\int \mathrm{d}\tau_3 O(\tau_1, \tau_3) G(\tau_3, \tau_2)}_{=m\left[-\frac{\partial^2}{\partial\tau_1^2}+\omega^2\right]G(\tau_1,\tau_2)} = \delta(\tau_1 - \tau_2), \quad G(\pm\beta/2, \tau_2) = 0 \text{ (Dirichlet B.C.)}$$

The Green's function G for the operator O with Dirichlet B.C. could be written $G_D(\tau_1, \tau_2)$, but it could be confused with the Dirichlet 2-point function that we defined in Lecture 5 (eq. 2.24). However, we will see later on that they are actually the same!

Using the shorthand notation

$$J \cdot G_D \cdot J \equiv \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2\, J(\tau_1) G_D(\tau_1, \tau_2) J(\tau_2), \tag{2.57}$$

we find

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

Exercise 2.3 (Green's function for the HO with Dirichlet B.C.)**.**
Consider the equations verified by the Green's function $G_D(\tau_1, \tau_2)$:

$$m\left[-\frac{\partial^2}{\partial\tau_1^2} + \omega^2\right] G_D(\tau_1, \tau_2) = \delta(\tau_1 - \tau_2), \qquad G_D(\pm\beta/2, \tau_2) = 0. \tag{2.59}$$

Show that

$$G_D(\tau_1, \tau_2) = \frac{1}{m\omega} \frac{\sinh\omega(\beta/2 + \tau_<)\sinh\omega(\beta/2 - \tau_>)}{\sinh\omega\beta}, \tag{2.60}$$

where $\tau_< = \min(\tau_1, \tau_2)$ and $\tau_> = \max(\tau_1, \tau_2)$.
Hint: integrate the differential equation for G_D with respect to τ_1 on the interval $[\tau_2 - \epsilon, \tau_2 + \epsilon]$, with infinitesimal ϵ in order to get a matching condition between two solutions, where one is defined on $\tau_1 < \tau_2$ and the other one on $\tau_1 > \tau_2$.

The same reasoning as for $K_E[\beta, J]$ allows us to compute $Z[\beta, J]$:

$$\boxed{Z[\beta, J] = Z[\beta, 0]e^{\frac{1}{2\hbar}J\cdot G_P\cdot J} = \frac{1}{2\sinh(\omega\beta/2)}e^{\frac{1}{2\hbar}J\cdot G_P\cdot J}} \tag{2.61}$$

where G_P is the Green's function with **periodic B.C.**:

$$m\left[-\frac{\partial^2}{\partial\tau_1^2}+\omega^2\right]G_P(\tau_1,\tau_2)=\delta(\tau_1-\tau_2), \qquad \begin{cases} G_P(-\beta/2,\tau_2)=G_P(\beta/2,\tau_2) \\ \partial_{\tau_1}G_P(-\beta/2,\tau_2)=\partial_{\tau_1}G_P(\beta/2,\tau_2) \end{cases}.$$

This gives

$$G_P(\tau_1,\tau_2)=\frac{1}{2m\omega}\frac{\cosh\omega\left(\frac{\beta}{2}-|\tau_1-\tau_2|\right)}{\sinh\frac{\omega\beta}{2}} \tag{2.62}$$

The periodic boundary conditions that we impose on G_P can be understood as follows. Consider the function $f(\tau_1)\equiv G_P(\tau_1,\tau_2)$. This function $f(\tau_1)$ is defined on $[-\beta/2,\beta/2]$, and has the same value and derivative at the boundaries. We can therefore "curl up" the interval into a circle, where the boundary points $-\beta/2$ and $\beta/2$ are identified. The function $f(\tau_1)$ is completely smooth on the circle since it is smooth when crossing from $-\beta/2$ to $\beta/2$.

An important property of both Green's functions G_D and G_P is their behaviour as $\beta\to\infty$:

$$\lim_{\beta\to\infty}G_D(\tau_1,\tau_2)=\lim_{\beta\to\infty}G_P(\tau_1,\tau_2)=\frac{1}{2m\omega}e^{-\omega|\tau_1-\tau_2|} \tag{2.63}$$

Free n-point correlators

In QFT, the word "free" means that there are no interactions, and the action is therefore Gaussian. In quantum physics, this is just the usual harmonic oscillator. Recall that

$$\hbar^{n/2}G_P(\tau_1,\ldots,\tau_n)=\frac{\hbar^n}{Z[\beta,0]}\frac{\delta}{\delta J(\tau_1)}\cdots\frac{\delta}{\delta J(\tau_1)}Z[\beta,J]\Big|_{J=0} \tag{2.64}$$

$$\hbar^{n/2}G_D(\tau_1,\ldots,\tau_n)=\frac{\hbar^n}{K_E[\beta,0]}\frac{\delta}{\delta J(\tau_1)}\cdots\frac{\delta}{\delta J(\tau_1)}K_E[\beta,J]\Big|_{J=0}, \tag{2.65}$$

where at this point $G_D(\tau_1,\ldots,\tau_n)$ and $G_P(\tau_1,\ldots,\tau_n)$ are the n-point functions we defined in lecture 5 (equations 2.24 and 2.30), **not** the Green's functions from this lecture. However, as we hinted at previously, they will turn out to be the same when $n=2$, which is why we use the same notation for the two different concepts. Recall also that

$$Z[\beta,J]=Z[\beta,0]e^{\frac{1}{2\hbar}J\cdot G_P\cdot J} \tag{2.66}$$

$$K_E[\beta,J]=K_E[\beta,0]e^{\frac{1}{2\hbar}J\cdot G_D\cdot J}, \tag{2.67}$$

where now in the exponential we have the Green's functions we computed in equations (2.60) and (2.62). Since J is an arbitrary function, we are free to rescale it as $J \to \sqrt{\hbar}J$, which leads to

$$G\left(\tau_1, \ldots, \tau_n\right) = \frac{\delta}{\delta J(\tau_1)} \cdots \frac{\delta}{\delta J(\tau_n)} e^{\frac{1}{2} J \cdot G \cdot J} \Big|_{J=0} \tag{2.68}$$

where now G can be either G_P or G_D. At this point we introduce a **graphical notation** to compute the n derivatives acting on the exponential. Let

$$\frac{1}{2} \int \mathrm{d}\tau_1 \mathrm{d}\tau_2 J(\tau_1) G(\tau_1, \tau_2) J(\tau_2) = \quad \otimes\!\!-\!\!-\!\!-\!\!\otimes \tag{2.69}$$

$$\int \mathrm{d}\tau_2 G(\tau_1, \tau_2) J(\tau_2) = \ \tau_1 \bullet\!\!-\!\!-\!\!-\!\!\otimes \tag{2.70}$$

$$G(\tau_1, \tau_2) = \ \tau_1 \bullet\!\!-\!\!-\!\!-\!\!\bullet\ \tau_2 \tag{2.71}$$

The reason why this notation is helpful is because it represents how derivatives act on the integral in the exponential:

$$\frac{\delta}{\delta J(\tau_1)} \quad \otimes\!\!-\!\!-\!\!-\!\!\otimes \ = \ \tau_1 \bullet\!\!-\!\!-\!\!-\!\!\otimes \tag{2.72}$$

$$\frac{\delta}{\delta J(\tau_2)} \ \tau_1 \bullet\!\!-\!\!-\!\!-\!\!\otimes = \ \tau_1 \bullet\!\!-\!\!-\!\!-\!\!\bullet\ \tau_2 \tag{2.73}$$

In addition to this property, we see from equation (2.68) that we must set $J = 0$ after taking the derivatives. **When $J = 0$, any $\otimes$ is 0**. Furthermore, the "direction" of a diagram does not matter:

$$\tau_1 \bullet\!\!-\!\!-\!\!-\!\!\otimes = \otimes\!\!-\!\!-\!\!-\!\!\bullet\ \tau_1 \ , \qquad \tau_1 \bullet\!\!-\!\!-\!\!-\!\!\bullet\ \tau_2 \ = \ \tau_2 \bullet\!\!-\!\!-\!\!-\!\!\bullet\ \tau_1 \tag{2.74}$$

We are now ready to prove that the 2 point functions $G_D(\tau_1, \tau_2)$ and $G_P(\tau_1, \tau_2)$ (left-hand side of eq. 2.68) are the same as the Green's functions $G_D(\tau_1, \tau_2)$ and $G_P(\tau_1, \tau_2)$ (right-hand side of eq. 2.68):

$$G(\tau_1, \tau_2) = \frac{\delta}{\delta J(\tau_1)} \frac{\delta}{\delta J(\tau_2)} e^{\frac{1}{2} J \cdot G \cdot J} \Big|_{J=0} \tag{2.75}$$

$$= \frac{\delta}{\delta J(\tau_1)} \Big(\ \tau_2 \bullet\!\!-\!\!-\!\!-\!\!\otimes \ \cdot e^{\frac{1}{2} J \cdot G \cdot J} \Big) \Big|_{J=0} \tag{2.76}$$

$$= \Big(\ \tau_2 \bullet\!\!-\!\!-\!\!-\!\!\bullet\ \tau_1 \ + \ \tau_2 \bullet\!\!-\!\!-\!\!-\!\!\otimes \ \cdot \ \tau_1 \bullet\!\!-\!\!-\!\!-\!\!\otimes \Big) \cdot e^{\frac{1}{2} J \cdot G \cdot J} \Big|_{J=0} \tag{2.77}$$

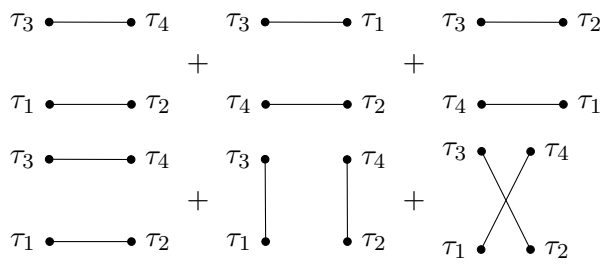
$$= \ \tau_2 \bullet\!\!-\!\!-\!\!-\!\!\bullet\ \tau_1 \tag{2.78}$$

$$= G(\tau_1, \tau_2). \tag{2.79}$$

Our notation for the Green's function is therefore justified.

A similar graphical computation can show us that any n-point function with n odd is 0, as there will always be a $\otimes$ left in one of the diagrams. The interesting computation is the 4-point function:

$$G(\tau_1,\tau_2,\tau_3,\tau_4) = \frac{\delta}{\delta J(\tau_1)}\frac{\delta}{\delta J(\tau_2)}\Big(\ \tau_3 \bullet\!\!-\!\!-\!\!\bullet \tau_4 \ +\ \tau_3 \bullet\!\!-\!\!-\!\!\otimes \ \cdot\ \tau_4 \bullet\!\!-\!\!-\!\!\otimes\Big)\cdot e^{\frac{1}{2}J\cdot G\cdot J}\Big|_{J=0}$$



$$= G(\tau_1,\tau_2)G(\tau_3,\tau_4) + G(\tau_1,\tau_3)G(\tau_2,\tau_4) + G(\tau_1,\tau_4)G(\tau_2,\tau_3) \tag{2.80}$$

Wick's theorem

The previous computation for the 4-point function shows the way to generalize to arbitrary n:

$$G(\tau_1,\ldots,\tau_n) = \begin{cases} 0 & \text{if } n \text{ is odd} \\ \displaystyle\sum_{p\in\sigma(n)} G(\tau_{p(1)},\tau_{p(2)})\ldots G(\tau_{p(n-1)},\tau_{p(n)}) & \text{if } n \text{ is even} \end{cases} \tag{2.81}$$

where $\sigma(n)$ is the group of permutations of n elements where the permutation of two elements in a pair ($G(\tau_i,\tau_j) = G(\tau_j,\tau_i)$) and the permutation of two pairs ($G(\tau_1,\tau_2)G(\tau_3,\tau_4) = G(\tau_3,\tau_4)G(\tau_1,\tau_2)$) is identified. It is useful to know the number of terms in the sum over the permutations in (eq. 2.81). We have

$$\binom{\text{number of permutations}}{p\in\sigma(n)} = \frac{n!}{(n/2)!2^{n/2}} = (n-1)!! = (n-1)(n-3)(n-5)\ldots \tag{2.82}$$

Equation (2.81) is known in QFT as **Wick's theorem**.

Note that what we did above was specific to the harmonic oscillator. Indeed, being able to factorize

$$Z[\beta,J] = Z[\beta,0]e^{\frac{1}{2}J\cdot G\cdot J}$$

is entirely dependent on the fact that the path integral is Gaussian. Even the Green's functions G_P and G_D were found for the specific case of the harmonic oscillator, since they were the inverse of the operator $O(\tau_1,\tau_2)$.

Summary of Lecture 6

- Propagators as functional derivatives of the system with a source:

$$\hbar^{n/2} G_P(\tau_1, \ldots, \tau_n) = \frac{\hbar^n}{Z[\beta, 0]} \frac{\delta}{\delta J(\tau_1)} \cdots \frac{\delta}{\delta J(\tau_1)} Z[\beta, J]\Big|_{J=0}$$
$$\hbar^{n/2} G_D(\tau_1, \ldots, \tau_n) = \frac{\hbar^n}{K_E[\beta, 0]} \frac{\delta}{\delta J(\tau_1)} \cdots \frac{\delta}{\delta J(\tau_1)} K_E[\beta, J]\Big|_{J=0}$$

- Forced harmonic oscillator:

$$Z_0[\beta, J] = Z_0[\beta, 0] e^{\frac{1}{2\hbar} J \cdot G_P \cdot J}, \quad G_D(\tau_1, \tau_2) = \frac{1}{m\omega} \frac{\sinh \omega(\beta/2 + \tau_<) \sinh \omega(\beta/2 - \tau_>)}{\sinh \omega\beta}$$
$$K_{E,0}[\beta, J] = K_{E,0}[\beta, 0] e^{\frac{1}{2\hbar} J \cdot G_D \cdot J}, \quad G_P(\tau_1, \tau_2) = \frac{1}{2m\omega} \frac{\cosh \omega\left(\frac{\beta}{2} - |\tau_1 - \tau_2|\right)}{\sinh \frac{\omega\beta}{2}}$$

- Wick's theorem:

$$G(\tau_1, \ldots, \tau_n) = \begin{cases} 0 & \text{if } n \text{ is odd} \\ \displaystyle\sum_{p \in \sigma(n)} G(\tau_{p(1)}, \tau_{p(2)}) \ldots G(\tau_{p(n-1)}, \tau_{p(n)}) & \text{if } n \text{ is even} \end{cases}$$

Lecture 7 - Feynman diagrams

Lecture 6 focused on deriving results for the harmonic oscillator. However, we would like to expand our methods to more general systems, where the action does not only contain quadratic terms. As you might expect, these more complicated systems will not be solvable exactly, but they will be tractable when assuming that the deviation from the HO is small.

Perturbation theory

Consider the case of the anharmonic oscillator, where

$$V(x) = \frac{1}{2}m\omega^2 x^2 + \Delta V(x). \tag{2.83}$$

$\Delta V(x)$ could, for example, be a quartic term like λx^4. If we denote the lagrangian of the unperturbed HO by $\mathcal{L}_0$, the partition function of the perturbed system can be written as

$$\begin{aligned} Z[\beta, J] &= \int \mathcal{D}_E[x] \exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \left[\mathcal{L}_{E,0} - x(\tau)J(\tau) + \Delta V(x)\right]\right) \\ &= \int \mathcal{D}_E[x] \underbrace{\exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, \Delta V(x)\right)}_{W} \exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \left[\mathcal{L}_{E,0} - x(\tau)J(\tau)\right]\right). \end{aligned} \tag{2.84}$$

Expanding the exponential, we find

$$W = \sum_{k=0}^{\infty} \frac{1}{k!}\left(-\frac{1}{\hbar}\right)^k \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_k\, \Delta V(x(\tau_1)) \ldots \Delta V(x(\tau_k)). \tag{2.85}$$

Since we assume $\Delta V(x)$ to be some polynomial in x, we see that W will in fact be a sum of terms with a certain number of $x(\tau_1)$, a certain number of $x(\tau_2)$, etc... However, one can replace these $x(\tau_i)$ by $\hbar\frac{\delta}{\delta J(\tau_i)}$, since this derivative acting on the exponential on the right will bring down factors of $x(\tau_i)$. We therefore can replace

$$W \to \frac{1}{k!}\left(-\frac{1}{\hbar}\right)^k \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_k\, \Delta V\left(\hbar\frac{\delta}{\delta J(\tau_1)}\right) \ldots \Delta V\left(\hbar\frac{\delta}{\delta J(\tau_k)}\right). \tag{2.86}$$

At this point, since this sum does not depend on x anymore, we can bring the sum outside the path integral and convert it back to an exponential. We therefore have

$$Z[\beta, J] = \exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, \Delta V\left(\hbar\frac{\delta}{\delta J(\tau)}\right)\right) \underbrace{\int \mathcal{D}[x] \exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \left[\mathcal{L}_{E,0} - x(\tau)J(\tau)\right]\right)}_{\equiv Z_0[\beta,J]}$$

This decomposition is useful because we have compute $Z_0[\beta, J]$ in the previous section! After rescaling $J \to \sqrt{\hbar}J$ as before, we find

$$Z[\beta, J] = Z_0[\beta, 0] \exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, \Delta V\left(\sqrt{\hbar}\frac{\delta}{\delta J(\tau)}\right)\right) e^{\frac{1}{2}J\cdot G_P \cdot J} \tag{2.87}$$

At this point, we can turn the source off **after** computing all the derivatives to get the partition function for the perturbed system:

$$\boxed{Z[\beta] = Z_0[\beta] \exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, \Delta V\left(\sqrt{\hbar}\frac{\delta}{\delta J(\tau)}\right)\right) e^{\frac{1}{2}J\cdot G_P\cdot J}\Big|_{J=0}} \tag{2.88}$$

Example: quartic perturbation
Consider

$$\Delta V(x) = \frac{1}{4!}\lambda_4 x^4, \tag{2.89}$$

where we assume that λ_4 is a small parameter. We can perform an expansion in λ_4 by expanding out the exponential in (eq. 2.88). In practice, if we consider the leading order in λ_4, we find

$$Z_{LO}[\beta] = Z_0[\beta]\left(1 - \hbar\int_{-\beta/2}^{\beta/2}\mathrm{d}\tau\,\frac{1}{4!}\lambda_4\frac{\delta^4}{\delta J(\tau)^4}\right) e^{\frac{1}{2}J\cdot G_P\cdot J}\Big|_{J=0} \tag{2.90}$$

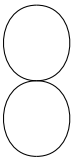
$$= Z_0[\beta]\left(1 - \frac{1}{4!}\hbar\lambda_4\int_{-\beta/2}^{\beta/2}\mathrm{d}\tau\;\frac{\delta^4}{\delta J(\tau)^4} e^{\frac{1}{2}J\cdot G_P\cdot J}\Big|_{J=0}\right) \tag{2.91}$$

Now in order to compute the derivatives, we can simply use Wick's theorem to get

$$\frac{\delta^4}{\delta J(\tau)^4} e^{\frac{1}{2}J\cdot G_P\cdot J}\Big|_{J=0} = 3G_P(\tau,\tau)^2, \tag{2.92}$$

or we could use the graphical notation, which would give

$$\frac{\delta^4}{\delta J(\tau)^4} e^{\frac{1}{2}J\cdot G_P\cdot J}\Big|_{J=0} = 3 \quad = 3G_P(\tau,\tau)^2. \tag{2.93}$$



The reason why there is a factor of 3 is because there are multiple equivalent ways to construct this diagram. One can think of starting with the point τ in the middle, out of which 4 legs come out (4 because we have 4 derivatives). Our task is to connect the 4 legs, which is essentially what Wick's theorem is about: we need to sum over each way of connecting the legs. Graphically, we pick one of the 4 legs, and we choose to connect it with one of the 3 remaining ones: that gives 3 possibilities. Then the last two legs have no choice but to be paired together. Therefore, the multiplicity of this diagram is 3, which is the same as the number of terms in the sum of Wick's theorem in this case (see eq. (2.82)).

Using this result, the partition function for the perturbed harmonic oscillator at leading order in λ is

$$Z_{LO}[\beta] = Z_0[\beta]\left(1 - \frac{1}{8}\hbar\lambda_4\int_{-\beta/2}^{\beta/2}\mathrm{d}\tau\, G_P(\tau,\tau)^2\right). \tag{2.94}$$

The integral can be done easily by using the definition of the periodic Green's function from equation (2.62):

$$Z_{LO}[\beta] = Z_0[\beta]\left(1 - \frac{1}{32}\frac{\hbar\beta\lambda_4}{m^2\omega^2}\coth^2\left(\frac{\omega\beta}{2}\right)\right). \tag{2.95}$$

Before going further with the quartic perturbation example, we can study another object from statistical mechanics: the **free energy** $F(\beta)$. For our purposes, it is defined as

$$F(\beta) = -\frac{\hbar}{\beta}\ln(Z(\beta)) \Leftrightarrow Z(\beta) = e^{-\frac{\beta}{\hbar}F(\beta)} \tag{2.96}$$

Knowing the free energy allows us to extract the ground state energy of the system:

$$\lim_{\beta\to\infty} F(\beta) = E_0 \tag{2.97}$$

If we know the partition function in perturbation theory as in equation (2.95), we can compute the free energy and extract the ground state energy of the perturbed system (as an expansion in the small parameter describing the perturbation).

Going back to our quartic perturbation example, we find

$$F_{LO}(\beta) = -\frac{\hbar}{\beta}\ln(Z_0[\beta]) - \frac{\hbar}{\beta}\ln\left(1 - \frac{1}{32}\frac{\hbar\beta\lambda_4}{m^2\omega^2}\coth^2\left(\frac{\omega\beta}{2}\right)\right) \tag{2.98}$$

$$= \frac{\hbar\omega}{2} + \frac{\hbar}{\beta}\ln\left(1 - e^{-\omega\beta}\right) + \frac{\hbar}{\beta}\left(\frac{1}{32}\frac{\hbar\beta\lambda_4}{m^2\omega^2}\coth^2\left(\frac{\omega\beta}{2}\right)\right) \tag{2.99}$$

$$= \underbrace{\frac{\hbar\omega}{2}\left[1 + \frac{2}{\omega\beta}\ln\left(1 - e^{-\omega\beta}\right)\right.}_{=F_0(\beta)} + \underbrace{\left.\frac{1}{16}\frac{\hbar\lambda_4}{m^2\omega^3}\coth^2\left(\frac{\omega\beta}{2}\right)\right]}_{\text{perturbation}} \tag{2.100}$$

One can clearly identify here the **dimensionless coupling**:

$$\bar{\lambda} = \frac{\hbar\lambda_4}{m^2\omega^3} \tag{2.101}$$

This dimensionless coupling is important because it is the number that regulates the validity of the perturbative expansion.

In the limit $\beta \to \infty$, we obtain the ground state energy of the system:

$$E_0 = \frac{\hbar\omega}{2}\left[1 + \frac{1}{16}\bar{\lambda} + \mathcal{O}(\bar{\lambda}^2)\right] \tag{2.102}$$

This result can be checked using the usual time-independent perturbation theory methods:

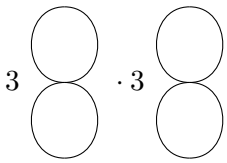
$$E_0 = \frac{\hbar\omega}{2} + \langle 0|\,\frac{\lambda_4}{4!}x^4\,|0\rangle + \mathcal{O}(\lambda_4^2) \tag{2.103}$$

We now consider the next order in perturbation theory. The order λ_4^2 is

$$\frac{1}{2!}\left(-\frac{\hbar\lambda_4}{4!}\right)^2 \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2 \, \frac{\delta^4}{\delta J(\tau_1)^4} \frac{\delta^4}{\delta J(\tau_2)^4} e^{\frac{1}{2}J\cdot G_P \cdot J}\Bigg|_{J=0} \tag{2.104}$$

We now use the graphical notation to compute this. We have two vertices, τ_1 and τ_2, which both have 4 legs. Our task now is to connect these legs and to keep track of the associated combinatorial factors (= the multiplicities of the diagrams).

- The most obvious diagram is the **disconnected** diagram: just two copies of the one we found for the leading order case. We get

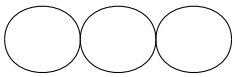


$$= 9G_P(\tau_1,\tau_1)^2 G_P(\tau_2,\tau_2)^2. \tag{2.105}$$

- Another diagram is to connect all 4 legs of the vertex τ_1 to the 4 legs of the vertex τ_2. There is $4! = 24$ ways to connect the legs, and we therefore get a factor

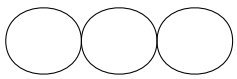
$$= 24\, G_P(\tau_1,\tau_2)^4 \tag{2.106}$$

- Lastly, we can do the hybrid case:



(2.107)

  The multiplicity of this diagram is a little bit harder. Consider one of the two vertices. We must choose 2 out of 4 legs to be connected with each other, which is equal to 6 possibilities. The same happens for the other vertex. Finally, the two remaining legs must connect to the two remaining legs of the other vertex, which gives an additional factor of 2 possibilities. This gives an overall multiplicity of $6 \cdot 6 \cdot 2 = 72$, and we therefore have a factor



$$= 72 \cdot G_P(\tau_1,\tau_1)^2 G_P(\tau_1,\tau_2)^2 G_P(\tau_2,\tau_2)^2$$

A useful trick to check that we did the combinatorics correctly is to compare the sum of the multiplicities of the diagrams to the number of terms in the sum in Wick's theorem, equation (2.82). In this case, we have

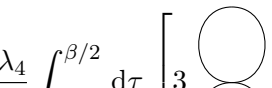
$$(8-1)!! = 7 \cdot 5 \cdot 3 = 105 = 9 + 24 + 72,$$

which is reassuring.

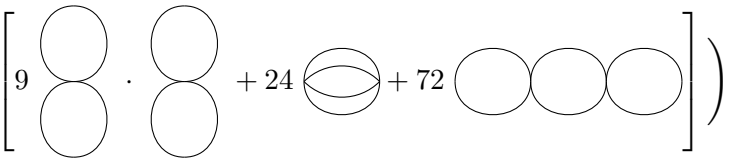
Free energy and connected diagrams

An important property of the free energy is that it can be completely written in terms of **connected diagrams**, unlike the partition function which contains **disconnected** diagrams. Before showing this in a general case, we compute the free energy to order λ_4^2 (next-to-leading order) in our quartic perturbation example:

$$Z_{NLO}(\beta) = Z_0[\beta]\Bigg(1 - \frac{\hbar\lambda_4}{4!}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau$$

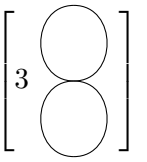


$$+ \frac{1}{2!}\left(-\frac{\hbar\lambda_4}{4!}\right)^2 \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2 \cdot$$

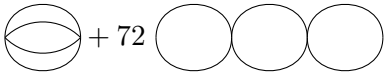


One can see here that the disconnected diagram term looks a lot like the leading order term squared. Actually, it is a general result that the partition function will be the **exponential of the connected diagrams**. Then, when we expand out the exponential, we get disconnected diagrams corresponding to the squares (or higher power) of the connected diagram. In our case, we can write

$$Z(\beta) = Z_0(\beta)\exp\Bigg(-\frac{\hbar\lambda_4}{4!}\int_{-\beta/2}^{\beta/2}\mathrm{d}\tau$$



$$+ \frac{1}{2!}\left(-\frac{\hbar\lambda_4}{4!}\right)^2 \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2$$



$$\Bigg) \tag{2.108}$$

We can get the free energy by taking the logarithm, and we therefore have the general result that

$$\boxed{F(\beta) = F_0(\beta) + \sum \text{connected diagrams}} \tag{2.109}$$

Exercise 2.4 (Second order corrections to the ground state energy)**.**
Compute the second order correction to the ground state energy for the perturbation $\Delta V(x) = \frac{\lambda_4}{4!}x^4$*. More specifically, find* c *in the equation*

$$E_0 = \frac{\hbar\omega}{2}\left[1 + \frac{1}{16}\bar{\lambda} + c\bar{\lambda}^2 + \mathcal{O}(\bar{\lambda}^3)\right]. \tag{2.110}$$

We present now two (non rigorous) arguments to convince ourselves that the free energy only cares about connected diagrams.

First argument:
Assume that the free energy does in fact only consist of connected diagrams. Then,

$$\frac{Z(\beta)}{Z_0(\beta)} = e^{-\frac{\beta}{\hbar}(F-F_0)} \sim e^{\sum_a C_a} \tag{2.111}$$

where a labels the different diagrams and C_a represents a connected diagram. Therefore,

$$\frac{Z(\beta)}{Z_0(\beta)} \sim \prod_a (1 + C_a + \frac{1}{2}C_a^2 + \ldots) \tag{2.112}$$

where now C_a^2 is a disconnected diagram made with 2 copies of C_a, just like in equation (2.105). We would also get different types of disconnected diagrams at higher order, such as a term C_aC_b where the disconnected diagram is two different connected diagrams. In our example, we did not encounter these but they would have appeared at order λ_4^3. It is fairly straightforward that the product over a becomes a sum over all possible diagrams (not only the connected ones). Our assumption that $F = F_0 + \sum_a C_a$ is therefore reasonable, since we found all diagrams in Z starting from only connected diagrams in F. This is not a complete proof since we have not verified that the coefficients in front of the diagrams also correspond.

Second argument:
Consider first a connected diagram, and study its dependency on β in the $\beta \to \infty$ limit:

$$\begin{pmatrix}\text{connected}\\ \text{diagram}\end{pmatrix} \sim \int \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_n \, f(\tau_1, \ldots, \tau_n), \tag{2.113}$$

where f is some function characterizing the diagram. Using time-translation invariance, we can set the origin of the time axis at τ_1, so that

$$\begin{pmatrix}\text{connected}\\ \text{diagram}\end{pmatrix} \sim \int \mathrm{d}\tau_1 \underbrace{\int \mathrm{d}\tau_2 \ldots \mathrm{d}\tau_n \, f(0, \tau_2, \ldots, \tau_n)}_{\text{converges as } \beta \to \infty} \sim \beta \tag{2.114}$$

The reason why the integral converges is that as $\beta \to \infty$, we have $G_P(\tau_i, \tau_j) \sim \frac{1}{2m\omega} e^{-\omega|\tau_i - \tau_j|}$, and therefore the integrand is exponentially suppressed as the separation between τ_i and τ_j increases.

Similarly, a disconnected diagram will scale as

$$\begin{pmatrix}\text{diagram with } k\\ \text{connected components}\end{pmatrix} \sim \begin{pmatrix}\text{connected}\\ \text{diagram}\end{pmatrix}^k \sim \beta^k \tag{2.115}$$

because a disconnected diagram is just the products of its connected components. Now, consider the free energy, and assume that it also contains disconnected diagrams. In that case, we would have

$$\begin{aligned} F(\beta) &= F_0(\beta) - \frac{\hbar}{\beta} \sum \text{diagrams} \\ &\xrightarrow{\beta\to\infty} \frac{\hbar\omega}{2} - \underbrace{\frac{\hbar}{\beta}\begin{pmatrix}\text{connected}\\ \text{diagram}\end{pmatrix}}_{\sim\beta^0} - \sum_{k=2}^{\infty} \underbrace{\frac{\hbar}{\beta}\begin{pmatrix}\text{diagram with } k\\ \text{connected components}\end{pmatrix}}_{\sim\beta^{k-1}} \end{aligned} \tag{2.116}$$

However, we know that $F(\beta) \xrightarrow{\beta\to\infty} E_0$, which is finite, therefore there cannot be disconnected diagrams in $F(\beta) - F_0(\beta)$.

We now present a **proof** of equation (2.109). Consider n decoupled copies of the same system. Then, the full partition function is the product of the initial system's partition function

$$Z_n(\beta) = [Z(\beta)]^n \implies F_n(\beta) = nF(\beta) \tag{2.117}$$

Perturbatively, we have

$$\frac{Z_n(\beta)}{[Z_0(\beta)]^n} = \exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \sum_{i=1}^{n} \Delta V\left(\sqrt{\hbar}\frac{\delta}{\delta J_i(\tau)}\right)\right) e^{\frac{1}{2}\sum_{i=1}^{n} J_i\cdot G_P\cdot J_i}\Bigg|_{J=0} \tag{2.118}$$

$$= 1 + n\sum\begin{pmatrix}\text{connected}\\ \text{diagrams}\end{pmatrix} + n^2\sum\begin{pmatrix}\text{diagrams with 2}\\ \text{connected components}\end{pmatrix} + \dots \tag{2.119}$$

We can then take the logarithm of the above to get

$$\ln\left(\frac{Z_n(\beta)}{[Z_0(\beta)]^n}\right) \approx n\sum\begin{pmatrix}\text{connected}\\ \text{diagrams}\end{pmatrix} + n^2\sum\begin{pmatrix}\text{diagrams with 2}\\ \text{connected components}\end{pmatrix} + \dots \tag{2.120}$$

since we are still doing perturbation theory (each diagram is "small compared to 1"). On the other hand, in terms of the free energy we have

$$\ln\left(\frac{Z_n(\beta)}{[Z_0(\beta)]^n}\right) \sim n(F(\beta) - F_0(\beta)) \tag{2.121}$$

Therefore,

$$n(F(\beta) - F_0(\beta)) \sim n\sum\begin{pmatrix}\text{connected}\\ \text{diagrams}\end{pmatrix} + \underbrace{\sum_{k=2}^{\infty} n^k \sum\begin{pmatrix}\text{diagrams with } k\\ \text{connected components}\end{pmatrix}}_{\text{these must vanish!}}, \tag{2.122}$$

where we identify terms with equal powers of n on both sides of the equation. We have now proven that

$$F(\beta) - F_0(\beta) \sim \sum\begin{pmatrix}\text{connected}\\ \text{diagrams}\end{pmatrix}. \tag{2.123}$$

Summary of Lecture 7

- Perturbation theory:

$$Z[\beta] = Z_0[\beta]\exp\left(-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, \Delta V\left(\sqrt{\hbar}\frac{\delta}{\delta J(\tau)}\right)\right) e^{\frac{1}{2}J\cdot G_P\cdot J}\Bigg|_{J=0}$$

- Free energy:

$$F(\beta) = -\frac{\hbar}{\beta}\ln(Z(\beta)), \quad \lim_{\beta\to\infty} F(\beta) = E_0$$

- Disconnected diagrams exponentiate:

$$F(\beta) = F_0(\beta) + \sum \text{connected diagrams}$$

Chapter 3

Non-perturbative effects

Lecture 8 - The semiclassical and fixed energy propagators

When the wavelength λ of a particle is much shorter than the typical length L over which the potential varies, we expect the dynamics to be well described by the classical motion. Indeed, 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. This is analogous to the geometric optics limit of the propagation of EM waves.

We have already seen in the previous chapter a method to analytically deal with systems that cannot be solved exactly: perturbation theory, with the use of Feynman diagrams. This method was only valid when the perturbation was small. In this chapter, we present another approximation, the **semiclassical approximation**. It corresponds to the limit $\hbar \to 0$, or more precisely

$$\frac{\lambda}{L} = \frac{\hbar}{p}\frac{V'}{V} \ll 1. \tag{3.1}$$

Note that these methods do not have a diagrammatic representation: when a small coupling g is involved, semiclassical contributions are typically proportional to $e^{-1/g}$. For example, we will see in lecture 10 that the separation between the ground state energy E_0 and the first excited state energy E_1 in the double well potential can be computed using semiclassical methods, which give the following energy splitting:

$$E_1 - E_0 \propto e^{-2/g} \tag{3.2}$$

where g is a dimensionless coupling. These effects vanish faster than any power of g when $g \to 0$ and thus they are called **non-perturbative corrections**.

The semiclassical propagator

Recall the definition of the propagator in Minkowski space:

$$K(x_f, t_f; x_i, t_i) = \int \mathcal{D}[x] e^{\frac{i}{\hbar}S[x]}. \tag{3.3}$$

We would like to study its behavior in the limit "$\hbar \to 0$". To do so, consider the change of variable $x(t) \to x'(t) = x_c(t) + \sqrt{\hbar} y(t)$, where $x_c(t)$ is the classical trajectory, found by solving the classical equation of motion

$$\left.\frac{\delta S}{\delta x}\right|_{x=x_c} = 0. \tag{3.4}$$

In the approximation of small $\hbar$, we can Taylor expand the action

$$S[x_c + \sqrt{\hbar} y] = S[x_c] + \int \mathrm{d}t_1 \mathrm{d}t_2 \; \frac{1}{2} \left.\frac{\delta^2 S}{\delta x^2}\right|_{x=x_c} \sqrt{\hbar} y(t_1) \sqrt{\hbar} y(t_2) + \mathcal{O}(\hbar^{3/2} y^3) \tag{3.5}$$

where the first order variation vanishes since x_c is the classical solution. Therefore, we obtain [1]

$$K(x_f, t_f; x_i, t_i) = e^{\frac{i}{\hbar} S[x_c]} \int \mathcal{D}[y] e^{\frac{i}{2} \left.\frac{\delta^2 S[x]}{\delta x^2}\right|_{x=x_c} y^2 + \mathcal{O}(\sqrt{\hbar} y^3)}, \tag{3.6}$$

It is then natural to define the **semiclassical propagator** as the propagator from (eq. 3.6) without the $\mathcal{O}(\sqrt{\hbar} y^3)$:

$$K_{sc}(x_f, t_f; x_i, t_i) = e^{\frac{i}{\hbar} S[x_c]} I[x_c], \tag{3.7}$$

$$\text{where } I[x_c] = \int \mathcal{D}[y] e^{\frac{i}{2} \int \mathrm{d}t_1 \mathrm{d}t_2 \left.\frac{\delta^2 S[x]}{\delta x(t_1) \delta x(t_2)}\right|_{x=x_c} y(t_1) y(t_2)}. \tag{3.8}$$

If we consider the specific example

$$S[x] = \int_{t_i}^{t_f} \mathrm{d}t \left[\frac{1}{2} m \dot{x}^2 - V(x)\right], \tag{3.9}$$

we find

$$I[x_c] = \int \mathcal{D}[y] e^{\frac{i}{2} \int \mathrm{d}t \left[m \dot{y}^2 - \Omega^2(t) y^2\right]}, \quad \Omega^2(t) \equiv V''(x_c(t)) \tag{3.10}$$

Notice that we have found a closed form expression for $I[x_c]$ with the Gelfand-Yaglom formula (1.107). Therefore, we can write

$$I[x_c] = e^{-i\frac{\pi}{2} n_-} \sqrt{\frac{m}{2\pi i \hbar |\psi_0(t_f)|}}, \tag{3.11}$$

$$\text{where } \left[-m\partial_t^2 - \Omega^2(t)\right] \psi_0(t) = 0, \quad \begin{cases} \psi_0(t_i) = 0 \\ \dot{\psi}_0(t_i) = 1 \end{cases} \tag{3.12}$$

There is a lot to be said about this phase factor in front: it can be deduced in several ways, and we present in the appendix (B.3) different ways of thinking about it. In summary, we show that the number of negative eigenvalues n_- from the Gelfand-Yaglom formula is equal to the number of zeroes of $\psi_0(t)$. It is much easier to find the number of zeroes than to count the negative eigenvalues, which is why this connection is interesting.

[1] Notice that the jacobian associated to the change of integration variable from $x(t)$ to $y(t)$ is just a (divergent) constant.

Van Vleck–Pauli–Morette formula

The goal of this formula is to give an explicit expression for $\psi_0(t_f)$ in terms of the classical action S_c. The classical path, x_c, verifies the equation of motion

$$m\ddot{x}_c + V'(x_c) = 0 \tag{3.13}$$

Taking a derivative with respect to time, we find

$$m\ddot{v}_c + V''(x_c)v_c = 0, \quad v_c = \dot{x}_c \tag{3.14}$$

We now see that v_c and ψ_0 solve the same ODE (although with different boundary conditions). It is then possible to relate them using an auxiliary function, the **Wronskian**:

$$W(t) \equiv v_c(t)\dot{\psi}_0(t) - \dot{v}_c(t)\psi_0(t) = v_c^2(t)\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\psi_0(t)}{v_c(t)}\right) \tag{3.15}$$

The Wronskian is constant because of the equations of motion:

$$\dot{W}(t) = v_c(t)\ddot{\psi}_0(t) - \ddot{v}_c(t)\psi_0(t) \tag{3.16}$$

$$= -\frac{V''(x_c)}{m}\left[v_c(t)\psi_0(t) - v_c(t)\psi_0(t)\right] = 0 \tag{3.17}$$

Therefore, $W(t) = W(t_i) = v_c(t_i)$. This allows us to express $\psi_0(t_f)$ as a function of v_c:

$$\psi_0(t_f) = v_c(t_i)v_c(t_f)\int_{t_i}^{t_f}\mathrm{d}t\frac{1}{v_c^2(t)} \tag{3.18}$$

The goal now is to connect with the classical action S_c. At the end of lecture 3, we saw interesting relations between derivatives of the action and the energy E and the final momentum p_f:

$$\frac{\partial S_c}{\partial x_f} = p_f, \qquad \frac{\partial S_c}{\partial t_f} = -E \tag{3.19}$$

Note that

$$p_f = mv_f = m\sqrt{\frac{2}{m}(E - V(x_f))}, \qquad v_f \equiv v_c(t_f) \tag{3.20}$$

which implies

$$\frac{\partial^2 S_c}{\partial x_i \partial x_f} = \frac{\partial p_f}{\partial x_i} = \frac{\partial E}{\partial x_i}\sqrt{\frac{m}{2(E - V(x))}} = \frac{\partial E}{\partial x_i}\frac{1}{v_f}, \tag{3.21}$$

There is a trick to easily compute $\frac{\partial E}{\partial x_i}$. Take the derivative with respect to x_i of the following equation:

$$t_f - t_i = \int_{t_i}^{t_f}\mathrm{d}t = \int_{x_i}^{x_f}\frac{\mathrm{d}x}{v} = \int_{x_i}^{x_f}\frac{\mathrm{d}x}{\sqrt{\frac{2}{m}(E - V(x))}} \tag{3.22}$$

Obviously $t_f - t_i$ is independent of x_i, but both E and the lower bound on the integral on the right hand side depend on x_i. Therefore,

$$0 = -\frac{1}{\sqrt{\frac{2}{m}(E - V(x_i))}} - \frac{1}{m}\frac{\partial E}{\partial x_i}\int_{x_i}^{x_f} \mathrm{d}x \left(\frac{2}{m}(E - V(x))\right)^{-3/2} \tag{3.23}$$

$$= -\frac{1}{v_i} - \frac{1}{m}\frac{\partial E}{\partial x_i}\int_{x_i}^{x_f} \frac{\mathrm{d}x}{v^3} \tag{3.24}$$

$$\implies \frac{\partial E}{\partial x_i} = -\frac{m}{v_i \int_{x_i}^{x_f} \frac{\mathrm{d}x}{v^3}}, \tag{3.25}$$

Plugging this back into equation (3.21) and using equation (3.18), we find

$$\frac{\partial^2 S_c}{\partial x_i \partial x_f} = -\frac{m}{v_i v_f \int_{x_i}^{x_f} \frac{\mathrm{d}x}{v^3}} = -\frac{m}{\psi_0(t_f)} \tag{3.26}$$

The semiclassical propagator can therefore be written as

$$\boxed{K_{sc}(x_f, t_f; x_i, t_i) = e^{\frac{i}{\hbar}S[x_c]} e^{-i\frac{\pi}{2}n_-} \sqrt{\frac{1}{2\pi i\hbar}\left|\frac{\partial^2 S_c}{\partial x_i \partial x_f}\right|}} \tag{3.27}$$

This is the Van Vleck–Pauli–Morette formula.

The fixed energy propagator

The energy levels of a quantum system can also be found from the propagator, by using the **fixed energy propagator**

$$K(E; x_f, x_i) \equiv \lim_{\epsilon \to 0^+} \int_0^\infty \mathrm{d}t \ \langle x_f | \, e^{-i\frac{\hat{H} - E - i\epsilon}{\hbar}t} \, | x_i \rangle \,, \tag{3.28}$$

We will show that if we think of E as a complex number and $K(E; x_f, x_i)$ as a complex function of E, the energy levels are given by poles of this function, and the energy eigenstates are related to the residues. Furthermore, semiclassical methods can be used to find $K(E; x_f, x_i)$ in the limit of small $\hbar$, which in turn leads to finding approximate energy levels. The goal of this section is to understand the analytic structure of the fixed energy propagator, and to see how useful information about the system can be extracted from it.

Note that in the definition above, the $i\epsilon$ prescription is present to ensure the convergence of the integral when $t \to \infty$: the integrand vanishes at $t \to \infty$ for any small ϵ for real E. If we analytically continue to complex E, we must look at $\mathrm{Im}(E) > 0$ to avoid exponential growth at infinity. Furthermore, we are assuming the hamiltonian is time-independent.

Using the definition of the usual propagator $K(x_f, t; x_i, 0) = \langle x_f | \, e^{-\frac{i}{\hbar}\hat{H}t} \, | x_i \rangle$, we can express the above as

$$K(E; x_f, x_i) \equiv \int_{-\infty}^{\infty} \mathrm{d}t e^{\frac{i}{\hbar}Et}\theta(t) K(x_f, t; x_i, 0). \tag{3.29}$$

Note that the $i\epsilon$ prescription is implicit here. We see here that the fixed energy propagator can be interpreted as the fourier transform of the function $\theta(t)K(x_f, t; x_i, 0)$, which is called the **retarded propagator**.

Performing the integration explicitly in (eq. 3.28) gives us

$$K(E; x_f, x_i) = \lim_{\epsilon \to 0^+} \langle x_f | \frac{i\hbar}{E - \hat{H} + i\epsilon} | x_i \rangle , \tag{3.30}$$

Inserting a basis of energy eigenstates, we find

$$K(E; x_f, x_i) = i\hbar \sum_n \frac{\psi_n(x_f)\psi_n^*(x_i)}{E - E_n}. \tag{3.31}$$

Let us now think of E as a complex variable and study the analytic structure of $K(E; x_f, x_i)$. If $\hat{H}$ has a discrete spectrum, $K(E; x_f, x_i)$ has simple poles at the eigenvalues of $\hat{H}$ (the energy levels E_n). However, it is also possible that $\hat{H}$ has a continuous spectrum of eigenvalues, in which case a branch cut would appear in the complex E plane (see figure 3.1).

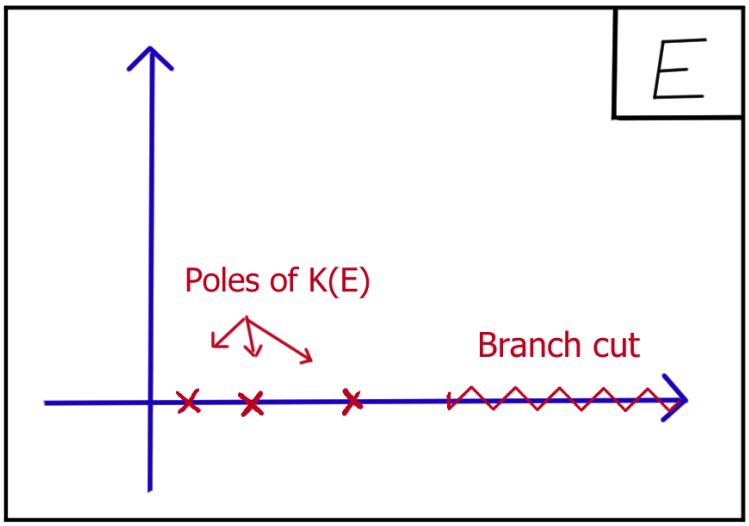


Figure 3.1: Analytic structure of $K(E; x_f, x_i)$ in the E-plane.

One can get significant information about energy levels by using this analytic structure. Indeed, consider the integral

$$\int_{-\infty}^{\infty} \mathrm{d}x \int_{C_\Lambda} \frac{\mathrm{d}E}{2\pi i} K(E; x, x), \tag{3.32}$$

where C_Λ is a contour in the complex plane that encircles all energy levels below a threshold value Λ (see figure 3.2). Here we are assuming a discrete energy spectrum.

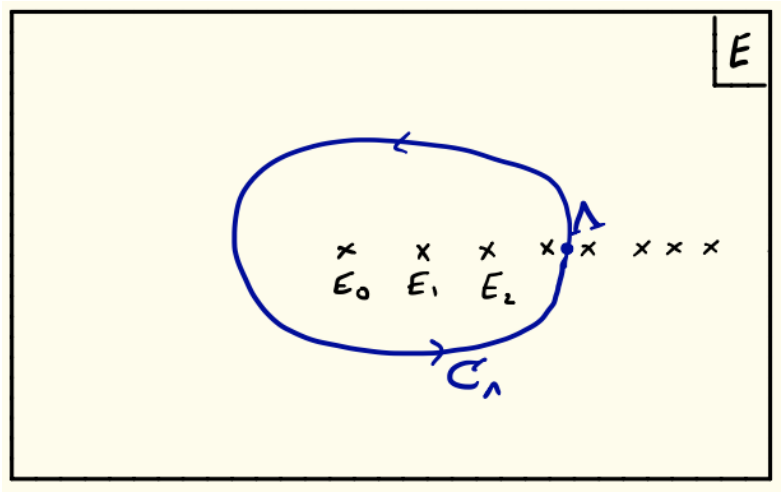


Figure 3.2: Contour of integration C_Λ in the E-plane picking up all the poles of $K(E; x_f, x_i)$ below $E = \Lambda$.

Using equation (3.31), we have

$$\int_{-\infty}^{\infty} \mathrm{d}x \int_{C_\Lambda} \frac{\mathrm{d}E}{2\pi i} K(E; x, x) = i\hbar \sum_n \int_{-\infty}^{\infty} \mathrm{d}x \, |\psi_n(x)|^2 \int_{C_\Lambda} \frac{\mathrm{d}E}{2\pi i} \frac{1}{E - E_n} \tag{3.33}$$

$$= i\hbar \sum_{E_n < \Lambda} 1 \equiv i\hbar\rho(\Lambda), \tag{3.34}$$

where we used the residue theorem (see A.2) to compute the integral over C_Λ. The function $\rho(\Lambda)$ is called the **integrated density of states**, and it counts how many states have energy below Λ.

How to compute $K(E; x_f, x_i)$?

In practice, how could we actually compute the fixed energy propagator? It turns out that it is the solution of a specific differential equation, which will be very close to the Schrödinger equation. To find this differential equation, define the operator

$$\hat{K} = \frac{i\hbar}{E - \hat{H} + i\epsilon} \tag{3.35}$$

such that

$$K(E; x_f, x_i) = \langle x_f | \, \hat{K} \, | x_i \rangle \,, \tag{3.36}$$

$$\lim_{\epsilon \to 0^+} (E - \hat{H} + i\epsilon)\hat{K} = i\hbar \tag{3.37}$$

Taking the matrix element of the left hand side of equation (3.37) between $\langle x|$ and $|y\rangle$ gives

$$\langle x| \lim_{\epsilon\to 0^+} (E - \hat{H} + i\epsilon)\hat{K} |y\rangle = \lim_{\epsilon\to 0^+} \left(E - \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right) + i\epsilon\right) \underbrace{\langle x| \hat{K} |y\rangle}_{=K(E;x,y)} \tag{3.38}$$

$$= -\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) - E\right) K(E;x,y) \tag{3.39}$$

The matrix element of the right hand side simply gives $i\hbar\delta(x-y)$, and we therefore get the differential equation

$$\boxed{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) - E\right) K(E;x,y) = -i\hbar\delta(x-y)} \tag{3.40}$$

This equation is very reminiscent of the kind of equation verified by Green's functions (see for example exercise (2.3)). To solve it, consider first the case where $x \neq y$. Since (3.40) is now a homogeneous second order differential equation, there are 2 linearly independent solutions $\psi_1(x)$, $\psi_2(y)$ verifying

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) - E\right) \psi_i(x) = 0 \quad i = 1,2 \tag{3.41}$$

For $x \neq y$, we can construct $K(E;x,y)$ out of these two solutions. However, when $x = y$, we have a **matching condition** which can be obtained by integrating (3.40) on a small interval centered around y:

$$-i\hbar = \int_{y-\delta}^{y+\delta} \mathrm{d}x(-i\hbar\delta(x-y)) \tag{3.42}$$

$$= \int_{y-\delta}^{y+\delta} \mathrm{d}x \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) - E\right) K(E;x,y) \tag{3.43}$$

$$\approx \int_{y-\delta}^{y+\delta} \mathrm{d}x \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right) K(E;x,y) \quad (\delta \ll 1) \tag{3.44}$$

$$\approx -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}K(E;x,y)\Big|_{y-\delta}^{y+\delta} \tag{3.45}$$

$$\implies \frac{2mi}{\hbar} = \frac{\partial}{\partial x}K(E;x,y)\Big|_{y+\delta} - \frac{\partial}{\partial x}K(E;x,y)\Big|_{y-\delta} \tag{3.46}$$

In other words, the derivative (with respect to x) of $K(E;x,y)$ has a discontinuity when $x \to y$. This discontinuity is a constant given by $\frac{2mi}{\hbar}$.

Now we can guess the form of $K(E;x,y)$:

$$K(E;x,y) = A\left(\theta(x-y)\psi_1(x)\psi_2(y) + \theta(y-x)\psi_1(y)\psi_2(x)\right), \tag{3.47}$$

where we will fix A using the matching condition (3.46). This is a solution of the differential equation for $x \neq y$ since in that case it is proportional to either $\psi_1(x)$ (if $x > y$) or $\psi_2(x)$ (if $x < y$). It is continuous at $x = y$ since we just switch from the first term above to the second when we cross from $x < y$ to $x > y$. Lastly, we must compute the discontinuity of the first derivative. Since the functions $\psi_{1,2}(y)$ are continuous, we therefore have (using equation (3.46))

$$\frac{2mi}{\hbar} = A(\underbrace{\psi_1'(y)\psi_2(y) - \psi_1(y)\psi_2'(y)}_{=W}) \implies A = \frac{2mi}{\hbar W}. \tag{3.48}$$

W is the Wronskian, which we saw already in the derivation of the VanVleck-Pauli-Morette formula (see 3.15). The Wronskian is a constant, which can be proved using the differential equation satisfied by $\psi_{1,2}$. In the end, we have the following formula for the fixed energy propagator:

$$\boxed{K(E;x,y) = \frac{2mi}{\hbar W}\left(\theta(x-y)\psi_1(x)\psi_2(y) + \theta(y-x)\psi_1(y)\psi_2(x)\right),} \tag{3.49}$$

where ψ_i are solutions to the differential equation (3.41).

In order to find these functions ψ_i, we need to know the appropriate boundary conditions that they verify. Equivalently, we can look at the boundary conditions of $K(E;x,y)$. These boundary conditions depend on the value of E, so for now we restrict ourselves to the case

$$E < \min_x V(x) \tag{3.50}$$

Then, equation (3.41) becomes

$$\frac{\partial^2}{\partial x^2}\psi_i(x) = \underbrace{-\frac{2m(E - V(x))}{\hbar^2}}_{>0}\psi_i(x), \tag{3.51}$$

from which we can see that $\psi_i(x)$ are exponentially decaying/growing functions when $x \to \pm\infty$. Furthermore, we know from (3.31) that $K(E;x,y)$ is not divergent as $x \to \pm\infty$, and we also know that for finite y,

$$\lim_{x\to+\infty} K(E;x,y) = \lim_{x\to+\infty} \frac{2mi}{\hbar W}\psi_1(x)\psi_2(y), \tag{3.52}$$

$$\lim_{x\to-\infty} K(E;x,y) = \lim_{x\to-\infty} \frac{2mi}{\hbar W}\psi_1(y)\psi_2(x) \tag{3.53}$$

so we must choose $\psi_1(x)$ to be exponentially decaying at $x \to +\infty$, while $\psi_2(x)$ must be exponentially decaying at $x \to -\infty$ in order to have a convergent $K(E;x,y)$. In equations,

$$\text{for } E < \min_x V(x), \quad \text{B.C.'s are } \begin{cases} \psi_1(x) \xrightarrow{x\to+\infty} 0 \\ \psi_2(x) \xrightarrow{x\to-\infty} 0 \end{cases} \tag{3.54}$$

Now that we have understood the theory, we can try out our formalism with some examples.

Examples

1. Free particle

We consider the case $V(x) = 0$, and $E < \min_x V(x) = 0$. The functions $\psi_i(x)$, $i = 1, 2$ can be found by solving equation (3.51) with the boundary conditions (3.54). We find

$$\psi_1(x) = A_1 e^{-\frac{\sqrt{-2mE}}{\hbar}x} \tag{3.55}$$

$$\psi_2(x) = A_2 e^{\frac{\sqrt{-2mE}}{\hbar}x} \tag{3.56}$$

The Wronskian can easily be computed:

$$W = \psi_1'(x)\psi_2(x) - \psi_1(x)\psi_2'(x) = -2A_1A_2\frac{\sqrt{-2mE}}{\hbar}, \tag{3.57}$$

and we therefore get

$$K(E; x, y) = -i\sqrt{\frac{m}{-2E}}\left(e^{-\frac{\sqrt{-2mE}}{\hbar}(x-y)}\theta(x-y) + e^{-\frac{\sqrt{-2mE}}{\hbar}(y-x)}\theta(y-x)\right) \tag{3.58}$$

$$= -i\sqrt{\frac{m}{-2E}}e^{-\frac{\sqrt{-2mE}}{\hbar}|x-y|} \tag{3.59}$$

It is now interesting to look at the analytic structure of this propagator in the complex E plane. It has a branch cut for positive, real E due to the function $\sqrt{-E}$. This was expected! Indeed, we know that a free quantum particle has continuous energy levels $E > 0$.

The above fixed energy propagator was found by considering negative, real E but we can analytically continue it to the whole complex plane except for the cut. We expect a qualitative difference between the continuation above the cut ($\mathrm{Im}(E) > 0$) or below the cut ($\mathrm{Im}(E) < 0$). As explained when we introduced the fixed energy propagator, we must look at $\mathrm{Im}(E) > 0$ to avoid exponential growth at infinity in general. This means that we are going **above** the cut: we must consider $E + i\epsilon$, $E > 0$ in (3.59) and use the standard square root branch cut prescription:

$$\sqrt{-E - i\epsilon} \xrightarrow{\epsilon\to 0} -i\sqrt{E} \tag{3.60}$$

$$\implies K_+(E; x, y) \equiv \sqrt{\frac{m}{2E}}e^{ik|x-y|}, \quad \left(k = \frac{\sqrt{2mE}}{\hbar} > 0\right) \tag{3.61}$$

This corresponds to

$$\psi_1(x) \propto e^{ikx}, \quad \psi_2(x) \propto e^{-ikx} \tag{3.62}$$

If we interpret $\psi_{1,2}$ as the wavefunctions of real particles, we see that (after re-introducing the time-dependence from the Schrödinger equation)

$$\psi_1(x, t) \propto e^{-i\frac{E}{\hbar}t + ikx} = e^{-i\frac{E}{\hbar}\left(t - \frac{\hbar k}{E}x\right)} \tag{3.63}$$

$$\psi_2(x, t) \propto e^{-i\frac{E}{\hbar}t - ikx} = e^{-i\frac{E}{\hbar}\left(t + \frac{\hbar k}{E}x\right)} \tag{3.64}$$

We can now see that **both** wavefunctions describe **outgoing** waves in the limits $x \to \infty$ for ψ_1 and $x \to -\infty$ for ψ_2. Now $K(E;x,y)$ is proportional to ψ_1 when $x \to \infty$ and to ψ_2 when $x \to -\infty$, therefore $K(E;x,y)$ always describes outgoing waves! To summarize, we had the physical $+i\epsilon$ prescription at the beginning, and the fixed energy propagator was the Fourier transform of the **retarded** propagator. We have shown here that this leads to outgoing waves. If instead we had continued below the cut, i.e. using a $-i\epsilon$ prescription (advanced propagator), we would have obtained incoming waves.

Remark:
We can compare this to electrodynamics: if we consider a distribution of charges, and we move them around, the physical electromagnetic waves will be flowing outwards. In electrodynamics, we also used retarded Green's functions to model this phenomena. Conversely, using an advanced propagator in electrodynamics corresponds to sending waves from the past to be absorbed by the moving charges, and having no waves in the future - this again matches with the "advanced" ($-i\epsilon$ prescription) discussed above.

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2. Barrier penetration
Consider now the case of a potential $V(x)$ which vanishes at $x \to \pm\infty$ and has a barrier somewhere on the x-axis (see figure 3.3). Let us now study the ψ_1 and ψ_2 for positive energies. From the free particle case, we know that $\psi_1(x)$ is a purely outgoing wave at $x \to +\infty$, so at $x \to -\infty$ it must be a superposition of incoming and outgoing waves[2]. Similarly, $\psi_2(x)$ is purely outgoing at $x \to -\infty$, and is a superposition of incoming and outgoing at $x \to +\infty$.

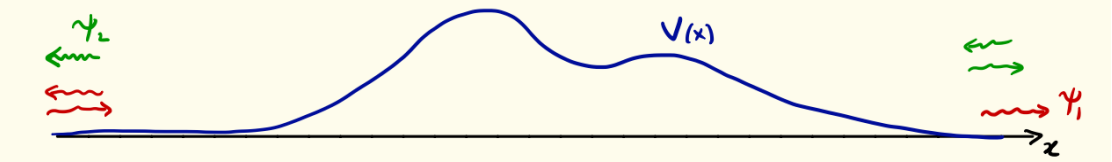


Figure 3.3: The potential barrier, and the wavefunctions ψ_1 and ψ_2.

In formulas, we can write

$$\psi_1(x) = \begin{cases} A_+ e^{ikx}, & x \to +\infty \\ e^{ikx} + B_+ e^{-ikx}, & x \to -\infty \end{cases}, \qquad \psi_2(x) = \begin{cases} B_- e^{ikx} + e^{-ikx}, & x \to +\infty \\ A_- e^{-ikx}, & x \to -\infty \end{cases}$$

Note that the overall normalization of the wavefunctions are not important since $K(E;x,y)$ is proportional to $\frac{\psi_1\psi_2}{W}$. Let us now compute the Wronskian:

$$W = \psi_1'\psi_2 - \psi_2'\psi_1 = \begin{cases} 2ikA_+, & x \to +\infty \\ 2ikA_-, & x \to -\infty \end{cases} \tag{3.65}$$

[2]There is a clear analogy with optics: these are the transmitted, incident and reflected waves.

This immediately tells us that $A_+ = A_- \equiv A$, since the Wronskian is a constant. Now A has a very clear physical interpretation: it is the transmission **amplitude**, from which we can get the transmission **probability**:

$$P_T = |A|^2 = \frac{W^2}{4k^2} \tag{3.66}$$

Is there a way that we could obtain this probability directly from the fixed energy propagator? To do so, let us look at the following limit:

$$\lim_{\substack{x\to+\infty \\ y\to-\infty}} K(E;x,y) = \lim_{\substack{x\to+\infty \\ y\to-\infty}} \frac{2mi}{\hbar W}\left(\theta(x-y)\psi_1(x)\psi_2(y) + \theta(y-x)\psi_1(y)\psi_2(x)\right) \tag{3.67}$$

$$= \lim_{\substack{x\to+\infty \\ y\to-\infty}} \frac{m}{\hbar k} A e^{ik(x-y)} \tag{3.68}$$

Therefore, the transmission amplitude A at energy E can be extracted from the limit $x \to \infty$, $y \to -\infty$ of the fixed energy propagator $K(E;x,y)$. In the next lecture, we will present a way to compute the fixed energy propagator in the semiclassical limit, and we will be able to look at the prefactor to deduce the transmission amplitude.

Summary of Lecture 8

- Semiclassical propagator:

$$K_{sc}(x_f,t_f;x_i,t_i) = e^{\frac{i}{\hbar}S[x_c]}\; e^{-i\frac{\pi}{2}n_-}\sqrt{\frac{m}{2\pi i\hbar|\psi_0(t_f)|}},$$

  $n_- = n_0$ is the number of negative eigenvalues of the operator $-\frac{\mathrm{d}^2}{\mathrm{d}t^2} - V''(x_c(t))$, or alternatively the number of zeroes of $\psi_0(t_f)$.

- The fixed energy propagator:

$$K(E;x,y) = \int_0^\infty \mathrm{d}t\; e^{\frac{i}{\hbar}Et} K(x_f,t_f;x_i,t_i) = i\hbar\sum_n \frac{\psi_n(x_f)\psi_n^*(x_i)}{E-E_n}$$

- Density of states:

$$\rho(\Lambda) = \sum_{E_n<\Lambda} 1 = \frac{1}{i\hbar}\int_{-\infty}^{\infty}\mathrm{d}x \oint_{C_\Lambda}\frac{\mathrm{d}E}{2\pi i}K(E;x,x)$$

- Barrier penetration:

$$K(E;x,y) \xrightarrow[y\to-\infty]{x\to+\infty} \frac{m}{\hbar k}Ae^{ik(x-y)}, \quad E = \frac{\hbar^2k^2}{2m} > 0,$$

  $|A|^2$ is the transmission probability at energy E.

Lecture 9 - The fixed energy propagator in the semiclassical limit

In lecture 8, we obtained the semiclassical approximation ("$\hbar \to 0$") of the propagator:

$$K_{sc}(x_f, t_f; x_i, t_i) = e^{\frac{i}{\hbar}S[x_c]}\ e^{-i\frac{\pi}{2}n_-}\sqrt{\frac{m}{2\pi i\hbar|\psi_0(t_f)|}},$$

Now the propagator itself appears in the definition of the fixed energy propagator (equation 3.29), so we can define the semiclassical fixed energy propagator as

$$K_{sc}(E; x_f, x_i) \equiv \int_0^\infty \mathrm{d}t\ e^{\frac{i}{\hbar}Et} K_{sc}(x_f, t; x_i, 0) \tag{3.69}$$

Then, using the VanVleck-Pauli-Morette formula (3.27) for K_{sc}, we can write

$$K_{sc}(E; x_f, x_i) = \int_0^\infty \mathrm{d}t\ e^{\frac{i}{\hbar}(S[x_c]+Et)} e^{-i\frac{\pi}{2}n_-}\sqrt{\frac{1}{2\pi i\hbar}\left|\frac{\partial^2 S_c}{\partial x_i \partial x_f}\right|} \tag{3.70}$$

Now in the semiclassical limit $\hbar \to 0$[3], we expect a saddle point approximation of the above integral to be valid.

Quick reminder of the saddle point approximation
Consider an integral of the form

$$I = \int_0^\infty \mathrm{d}t\ e^{\frac{i}{\hbar}g(t)} f(t) \tag{3.71}$$

In the limit $\hbar \to 0$, the complex exponential oscillates rapidly everywhere except at the extrema of $g(t)$, and the integral therefore "cancels out" in these regions (for much more detail, see exercise 10). Therefore, assuming only one minimum t_* for simplicity, we can approximate

$$I = e^{\frac{i}{\hbar}g(t_*)} f(t_*) \int_0^\infty \mathrm{d}t\ e^{\frac{i}{\hbar}\frac{1}{2}g''(t_*)(t-t_*)^2} \tag{3.72}$$

The integral above is approximately gaussian (one only needs to extend the integration domain to $(-\infty, \infty)$, which only brings a small error since the integral is dominated by the region near t_*). Performing the Gaussian integral, we find

$$I = e^{\frac{i}{\hbar}g(t_*)} f(t_*)\sqrt{\frac{2\pi i\hbar}{g''(t_*)}}(1 + \mathcal{O}(\hbar)) \tag{3.73}$$

We therefore need to find the saddle point t_* of $S[x_c] + Et$. Before computing t_*, it is important to understand which parameters are fixed and which are varied. E is an external fixed variable since we want to compute $K_{sc}(E; x_f, x_i)$. $S[x_c]$ is the action

[3] More rigorously, $S[x_c]/\hbar \gg 1$ and $E/\hbar \gg 1$

evaluated on the classical path, which is in turn determined by the boundary conditions: x_f, x_i and t. Therefore, the classical energy E_c also depends on the boundary conditions: $E_c \equiv E_c(x_f, t; x_i, 0)$.

One can think that given x_i and x_f fixed, there are different classical paths with different energies going from x_i to x_f in a time t. In the fixed-energy propagator, this time t is not fixed, which is why there can be many classical paths with different energies E_c.

Exercise 3.1 (Classical mechanics with boundary conditions)**.** *Consider a freely falling ball (under the action of a gravitational force* $\mathbf{F} = -mg\hat{x}$*) described by the classical path* $x_c(t)$*, with boundary conditions* $x_c(0) = x_i$ *and* $x_c(t_f) = x_f$*. Express* $x_c(t)$ *and* E_c *in terms of* x_i*,* x_f*,* t_f *and* g*. Do you see how different values of* t_f *lead to different* E_c*? Which path has the smallest* E_c*?*

Recall that at the end of lecture 3 we proved that $\partial_{t_f} S[x_c] = -E_c$ (equation 1.132). In our case, $t_f = t$ and $t_i = 0$. Therefore,

$$0 = \partial_t (S[x_c] + Et)|_{t=t_*} = -E_c(t_*) + E \tag{3.74}$$

The saddle point t_* is therefore the time such that $E_c = E$, i.e. the time it takes the classical particle to go from x_i to x_f with **fixed** energy E. There are cases where there might be multiple such points, which will be discussed later.

Single saddle point

To use the saddle point approximation, we still need to compute the second derivative. We have

$$\partial_t^2 (S[x_c] + Et)\big|_{t=t_*} = -\,\partial_t E_c|_{t=t_*} \tag{3.75}$$

Now there is a trick to easily find $\partial_t E_c$:

$$t = \int_{x_i}^{x_f} \frac{\mathrm{d}x}{\dot{x}} = \int_{x_i}^{x_f} \mathrm{d}x \, \sqrt{\frac{m}{2(E_c - V(x))}} \tag{3.76}$$

$$\implies 1 = \partial_t \int_{x_i}^{x_f} \mathrm{d}x \, \sqrt{\frac{m}{2(E_c - V(x))}} \tag{3.77}$$

$$= -\partial_t E_c \int_{x_i}^{x_f} \mathrm{d}x \, \frac{1}{m} \left(\frac{m}{2(E_c - V(x))} \right)^{-3/2}. \tag{3.78}$$

Therefore,

$$-\partial_t E_c = \frac{m}{\int_{x_i}^{x_f} \frac{\mathrm{d}x}{v^3}} \tag{3.79}$$

Now we have encountered the integral in the denominator before, during the derivation of the VanVleck-Pauli-Morette formula (eq. 3.26). We can use that result to obtain

$$-\partial_t E_c = -v_i v_f \frac{\partial^2 S_c}{\partial x_i \partial x_f} \tag{3.80}$$

We now have all the ingredients to compute the saddle point approximation of the fixed energy propagator:

$$K_{sc}(E; x_f, x_i) = \frac{1}{\sqrt{v_i v_f}} e^{\frac{i}{\hbar}(S[x_c]+Et)}\Big|_{t=t_*} \tag{3.81}$$

Lastly, we can write $(S[x_c] + Et)|_{t=t_*}$ in a simpler way:

$$S[x_c] = \int_0^t \mathrm{d}t\ \frac{1}{2} m\dot{x}^2 - V(x) \tag{3.82}$$

$$= \int_{x_i}^{x_f} \frac{\mathrm{d}x}{\dot{x}}\ (m\dot{x}^2 - E_c) \tag{3.83}$$

$$= -E_c t + \int_{x_i}^{x_f} \mathrm{d}x\ p(x), \quad (p = m\dot{x}) \tag{3.84}$$

Therefore, since $E_c(t_*) = E$, we have

$$\boxed{K_{sc}(E; x_f, x_i) = \frac{1}{\sqrt{v_i v_f}} e^{\frac{i}{\hbar}\int_{x_i}^{x_f} \mathrm{d}x\ p(x)}} \tag{3.85}$$

Note that this formula can be written as a product:

$$K_{sc}(E; x_f, x_i) = \psi_{\mathrm{WKB}}(x_f)\psi^*_{\mathrm{WKB}}(x_i), \tag{3.86}$$

where

$$\psi_{\mathrm{WKB}}(x) = \frac{1}{\sqrt{v(x)}} e^{\frac{i}{\hbar}\int_{x_0}^{x} \mathrm{d}x\ p(x)} \tag{3.87}$$

The value of x_0 is irrelevant to us since it cancels out in the formula for K_{sc}. Note that this is reminiscent of the formalism we had before taking the semiclassical limit with the wavefunctions ψ_1 and ψ_2 (see eq. 3.49). These WKB wavefunctions can be computed directly from the Schrödinger equation, which is done in exercise 24.

Before treating the case of multiple saddle points, we can analytically continue equation (3.85) to negative energies to compare with some analytical examples we computed in lecture 8. The velocities and momentum in the integral must be continued carefully. Recall that

$$v(x) = \sqrt{\frac{2(E - V(x))}{m}} \tag{3.88}$$

and that we must give a small imaginary part to the energy to fix the branch cut ambiguity. Therefore,

$$v(x) \xrightarrow{E<0} i\sqrt{\frac{2(V(x)-E)}{m}} \tag{3.89}$$

and we find

$$K_{sc}(E;x_f,x_i) = \frac{-i\sqrt{\frac{m}{2}}}{(V(x_i)-E)^{1/4}(V(x_f)-E)^{1/4}} e^{-\frac{1}{\hbar}\int_{x_i}^{x_f} \mathrm{d}x\, \sqrt{2m(V(x)-E)}}, \quad E<0 \tag{3.90}$$

The analytic structure of this expression is what we expected: for $E < \min_{x_i<x<x_f} V(x)$, all square roots have positive arguments, and the function is analytic. For larger E, there are branch cuts which reflect the continuous energy levels of the particle in the potential. At the exact level (not the semiclassical approximation we are working with here), we would expect a discrete spectrum. Intuitively, these discrete poles get closer and closer together as $\hbar \to 0$, until they become a branch cut in the semiclassical limit.

We would like to compare our semiclassical approximation to the analytic result for the free particle (eq. 3.59). The semiclassical approximation gives:

$$K_{sc}^{(\text{free})}(E;x_f,x_i) = -i\sqrt{\frac{m}{-2E}} e^{-\frac{\sqrt{-2mE}}{\hbar}(x_f-x_i)}, \tag{3.91}$$

which is the same expression as the analytic solution. In this case, the semiclassical approximation is exact!

Multiple saddle points

In the previous section, we considered the case of a single saddle point t_*. Could there be multiple different classical trajectories with fixed energy E, which take different times t_* to go from x_i to x_f? Consider the case where there is a "valley" in the potential, and the classical trajectories are oscillating in that valley, as shown in figure 3.4.

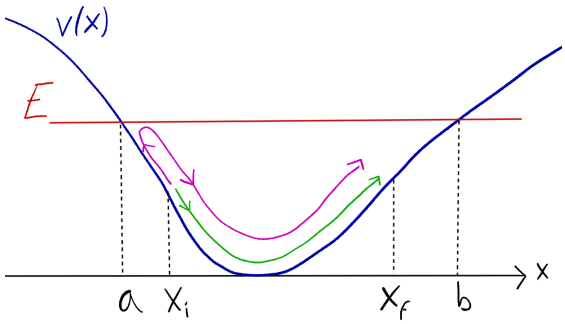


Figure 3.4: Two possible classical paths from x_i to x_f with energy E. The green path goes directly to x_f, while the pink path starts by reaching the turning point a and then goes to x_f.

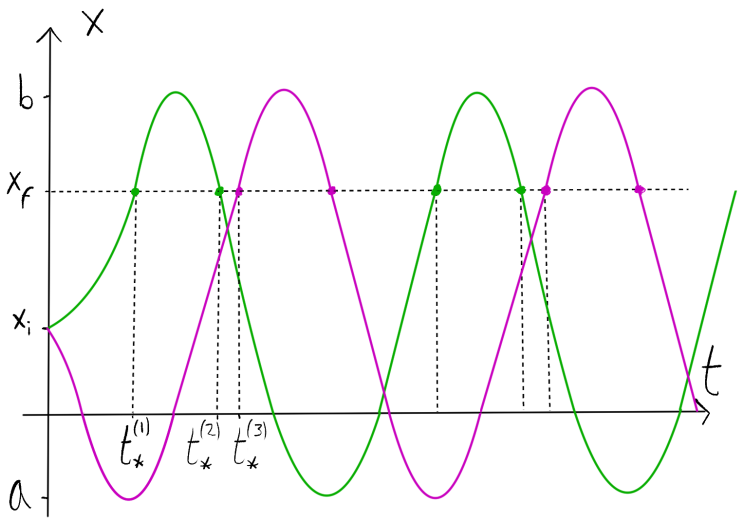


Figure 3.5: Two categories of path are shown: in green, the paths that initially go towards x_f, and in pink the paths initially going away from x_f. The saddle points $t_*^{(n)}$ are present whenever a path reaches x_f.

The paths oscillate between the turning points a and b where $V(a) = V(b) = E$. Now given $a \leq x_i,\ x_f \leq b$, there can be many paths going from x_i to x_f. First of all, the path can start by going towards x_f (shown in green) or away (in pink). There is an infinite number of saddle points since a path can oscillate arbitrarily many times between a and b. These paths are shown in figure 3.5, and we label them by the integer n.

We can now compute $K_{sc}(E; x_f, x_i)$ by summing over the saddle points. The first modification comes from the integral in the exponential: $\int_{x_i}^{x_f} \mathrm{d}x\, p(x)$ naively does not take into account the oscillation "history" of a path. To include it, we can write

$$\int_{x_i}^{x_f} \mathrm{d}x_{(n)}\, p(x) \equiv \int_0^{t_*^{(n)}} \mathrm{d}t\, m\dot{x}^2, \tag{3.92}$$

where $\mathrm{d}x_{(n)}$ is a notational tool to remind us to consider the "n"-th path. We would therefore have

$$K_{sc}(E; x_f, x_i) = \sum_n \frac{1}{\sqrt{v(x_i)v(x_f)}} e^{\frac{i}{\hbar}\int_{x_i}^{x_f} \mathrm{d}x_{(n)}\, p(x)} \tag{3.93}$$

Note however that $v(x_f)$ changes sign depending on which path we are considering. For example, if the simplest green path has $v(x_f) > 0$, but the second green path has $v(x_f) < 0$. These lead to complex phases, similar to the discussion "Phases from analytic continuation" of lecture 8. As explained previously, we should consider the times to have a small negative imaginary part, i.e. $t \to t - i\epsilon$. Therefore,

$$v(x_f) \to v(t_*^{(n)} - i\epsilon) = v(t_*^{(n)}) - i\epsilon \dot{v}(t_*^{(n)}) \tag{3.94}$$

Now $v(t)$ is an oscillatory function, and therefore $v(t_*^{(n)} - i\epsilon)$ goes counter-clockwise around the branch point ($v(x_f) = 0$) as n increases. For this reason, the rigorous formula for the semiclassical fixed energy propagator with multiple saddle points (for $E > 0$) is

$$\boxed{K_{sc}(E; x_f, x_i) = \sum_n \frac{e^{-i\frac{\pi}{2}N_n}}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\int_{x_i}^{x_f} \mathrm{d}x_{(n)}\, p(x)}}, \tag{3.95}$$

where N_n is the number of turning points (points where $v = 0$) for a given path labeled by n. For example, the simplest green path has $N_1 = 0$, the next one has $N_1 = 1$, and the simplest pink path (labelled by 3 in figure (3.5)) has $N_3 = 1$ as well.

Application 1: barrier penetration

Consider a potential that vanishes at $\pm\infty$ with a barrier somewhere on the x-axis, as in the example from lecture 8. We would like to compute the limit $x \to \infty$, $y \to -\infty$ of $K_{sc}(E; x, y)$ in order to extract the transmission probability in the semiclassical approximation. First, we consider negative E and we will then continue to physical energies. Using equation (3.90), we have

$$\lim_{\substack{x\to+\infty \\ y\to-\infty}} K_{sc}(E; x, y) = \lim_{\substack{x\to+\infty \\ y\to-\infty}} -i\sqrt{\frac{m}{-2E}} e^{-\frac{1}{\hbar}\int_y^x \mathrm{d}z\, \sqrt{2m(V(z)-E)}} \tag{3.96}$$

Now we go to physical energies, with the $+i\epsilon$ prescription to be above the cut

$$E \to \frac{\hbar^2 k^2}{2m} + i\epsilon \tag{3.97}$$

$$\implies \sqrt{-E} \to -i\frac{\hbar k}{\sqrt{2m}} \tag{3.98}$$

Therefore, for physical energies we have

$$\lim_{\substack{x\to+\infty \\ y\to-\infty}} K_{sc}(E; x, y) = \lim_{\substack{x\to+\infty \\ y\to-\infty}} \frac{m}{\hbar k} e^{-\frac{1}{\hbar}\int_y^x \mathrm{d}z\, \sqrt{2m(V(z)-E)}} \tag{3.99}$$

Now the integral in the exponential can be split into 5 different integration regions (see figure 3.6)

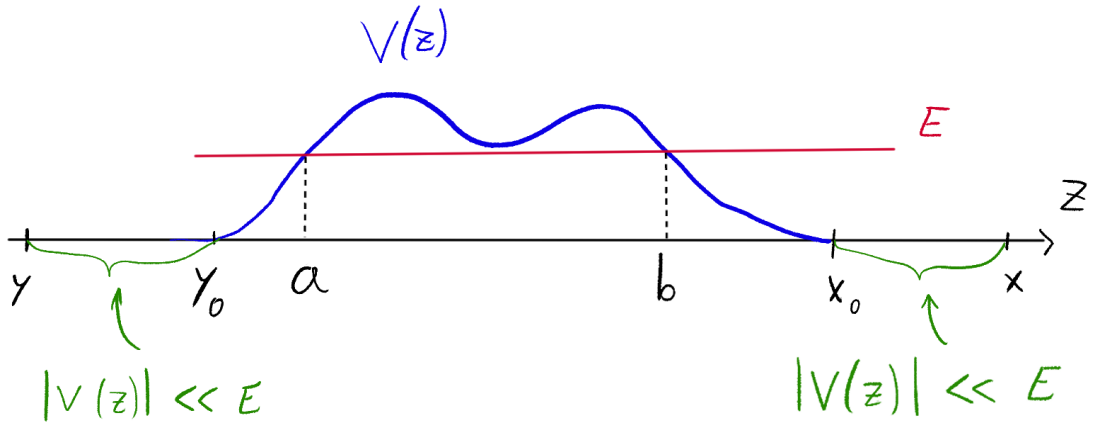


Figure 3.6: Definition of important regions of integration: $y_0 < z < x_0$ is the region where the potential cannot be neglected, while a and b are the classical turning points.

Let us first do the integrals on the extreme edges of the interval $[y, x]$:

$$\int_y^{y_0} \mathrm{d}z \, \sqrt{2m\left(V(z) - E\right)} = \sqrt{-2mE}(y_0 - y) = -i\hbar k(y_0 - y) \tag{3.100}$$

$$\int_{x_0}^{x} \mathrm{d}z \, \sqrt{2m\left(V(z) - E\right)} = \sqrt{-2mE}(x - x_0) = -i\hbar k(x - x_0) \tag{3.101}$$

Then, there are the integrals where $E > V(z)$ but $V(z)$ is not negligible:

$$\int_{y_0}^{a} \mathrm{d}z \, \sqrt{2m\left(V(z) - E\right)} = -i \int_{y_0}^{a} \mathrm{d}z \, \sqrt{2m\left(E - V(z)\right)} \tag{3.102}$$

$$\int_{b}^{x_0} \mathrm{d}z \, \sqrt{2m\left(V(z) - E\right)} = -i \int_{b}^{x_0} \mathrm{d}z \, \sqrt{2m\left(E - V(z)\right)} \tag{3.103}$$

Finally, there is the classically forbidden region between the turning points, where the integral does not need to be changed. We end up with

$$\lim_{\substack{x\to+\infty \\ y\to-\infty}} K_{sc}(E; x, y) = \lim_{\substack{x\to+\infty \\ y\to-\infty}} \frac{m}{\hbar k} \underbrace{e^{\frac{i}{\hbar}\Phi} e^{-\frac{1}{\hbar}\int_a^b \mathrm{d}z \, \sqrt{2m(V(z)-E)}}}_{=A} e^{ik(x-y)} \tag{3.104}$$

where we defined

$$\Phi = \int_{y_0}^{a} \mathrm{d}z \, \sqrt{2m\left(E - V(z)\right)} + \int_{b}^{x_0} \mathrm{d}z \, \sqrt{2m\left(E - V(z)\right)} + \hbar k(y_0 - x_0) \tag{3.105}$$

and A is the transmission amplitude, which we obtained by comparing with equation (3.68) from lecture 8. The value of Φ is irrelevant for physical probabilities since we want to compute the transmission probability $|A|^2$. We have therefore found an explicit expression for the transmission probability in the semiclassical approximation P_{sc}:

$$\boxed{P_{sc} = \exp\left(-\frac{2}{\hbar}\int_a^b \mathrm{d}z \, \sqrt{2m\left(V(z) - E\right)}\right)} \tag{3.106}$$

Application 2: spectral density

We would now like to use the semiclassical fixed energy propagator to get information about the energy levels. To do so, we will compute the semiclassical spectral density $\rho_{sc}(\Lambda)$. Recall that in lecture 8 (equation 3.34) we proved that

$$\rho(\Lambda) = \sum_{E_n<\Lambda} 1 = \frac{1}{i\hbar}\int_{-\infty}^{\infty} \mathrm{d}x \int_{C_\Lambda} \frac{\mathrm{d}E}{2\pi i} K(E;x,x), \tag{3.107}$$

where C_Λ was some contour that encircled all energy levels $E_n < \Lambda$. Now to adapt this to the semiclassical case, we have to be careful since $K_{sc}(E;x,x)$ has a branch cut for $E > V(x)$: using equation (3.90), we have

$$K_{sc}(E;x,x) = -i\sqrt{\frac{m}{2(V(x)-E)}}, \quad E<0 \tag{3.108}$$

since the integral in the exponential gives 0 when $x_i = x_f = x$.

There is a subtle issue associated with this branch cut. We are considering the case of a potential well (see figure 3.7), which means that the energy levels ($E > 0$) are discretized. However, our semiclassical approximation, when analytically continued to $E > 0$, gives us a continuous spectrum of energy levels corresponding to the branch cut. This subtlety comes from the fact that for positive E, we are in the case of multiple saddle points as described earlier. By simply taking the single saddle point K_{sc} with $E < 0$ and continuing it to $E > 0$, we are missing this subtlety and will therefore also miss the discrete nature of the energy spectrum. However, the answer we will get is a kind of "average" of the more precise solution obtained by using multiple saddle points, which is still relevant physically. The more complex discussion using multiple saddle points can be found in the appendix B.4. We will now present a method for finding ρ_{sc} in the case of a branch cut at $E > 0$.

Because of the branch cut, the integration contour C_Λ crosses the branch cut if $\Lambda > V(x)$ and the resulting integral is therefore ill-defined. To remedy this, consider approximating the original contour of integration in (3.107) by removing an infinitesimal interval near $E = \Lambda$, so that we do not cross the real axis (we are now considering an open contour, denoted $\tilde{C}_\Lambda$). At the exact level, i.e. before taking the semiclassical limit, this should not have a large effect on the result. However, it makes the semiclassical integration much more tractable. By deforming the contour (see figure 3.8), we can perform the integration for the semiclassical spectral density easily. We have

$$\rho_{sc}(\Lambda) \equiv -\frac{1}{\hbar}\sqrt{\frac{m}{2}}\int_{-\infty}^{\infty} \mathrm{d}x \int_{\bar{C}_\Lambda} \frac{\mathrm{d}E}{2\pi i} \frac{1}{\sqrt{V(x)-E}} \tag{3.109}$$

Now the integral over $\bar{C}_\Lambda$ can be done by summing the integral from Λ to $V(x)$ above the cut, denoted I_+, and the integral from $V(x)$ to Λ below the cut, denoted I_-. In practice,

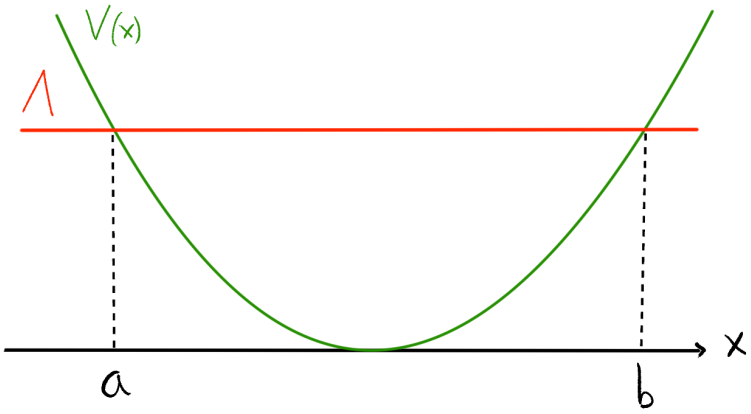


Figure 3.7: Potential well where a and b correspond to the turning points for a particle with energy Λ.

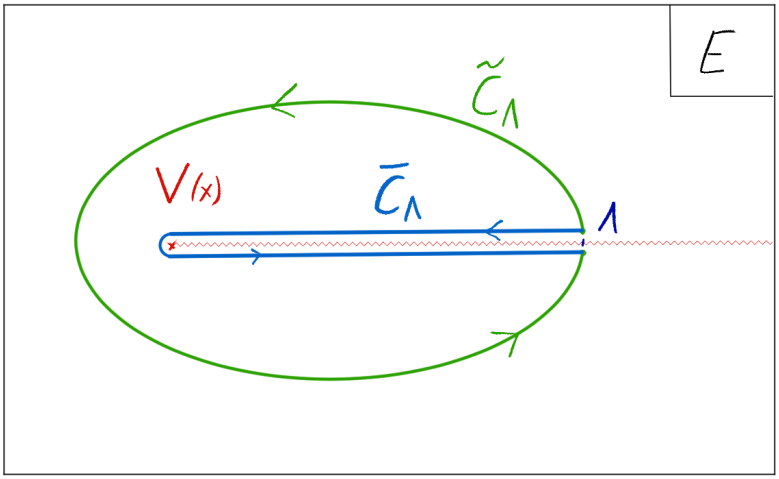


Figure 3.8: In red, the branch cut starting from $V(x)$. To avoid the branch cut, we remove the part of the contour C_Λ near $E = \Lambda$, giving us the new contour $\tilde{C}_\Lambda$. After deformation, we integrate over $\bar{C}_\Lambda$.

we have

$$I_+ = \int_\Lambda^{V(x)} \frac{\mathrm{d}E}{2\pi i} \frac{1}{\sqrt{V(x) - E - i\epsilon}} \tag{3.110}$$

$$= -i \int_{V(x)}^{\Lambda} \frac{\mathrm{d}E}{2\pi i} \frac{1}{\sqrt{E - V(x)}} \tag{3.111}$$

$$I_- = \int_{V(x)}^{\Lambda} \frac{\mathrm{d}E}{2\pi i} \frac{1}{\sqrt{V(x) - E + i\epsilon}} \tag{3.112}$$

$$= -i \int_{V(x)}^{\Lambda} \frac{\mathrm{d}E}{2\pi i} \frac{1}{\sqrt{E - V(x)}}, \tag{3.113}$$

so both integrals contribute the same. We end up with

$$\rho_{sc}(\Lambda) = \frac{2i}{\hbar}\sqrt{\frac{m}{2}} \int_{-\infty}^{\infty} \mathrm{d}x \int_{V(x)}^{\Lambda} \frac{\mathrm{d}E}{2\pi i} \frac{1}{\sqrt{E - V(x)}} \theta(\Lambda - V(x)), \tag{3.114}$$

where we added a theta function to ensure that $\Lambda > V(x)$. If we had considered $\Lambda < V(x)$, the spectral density would be 0 since the integrand would be analytic inside the contour (alternatively, there would be no discontinuity across the branch cut so I_+ and I_- would cancel out). Now, the rest of the computation is simple real analysis:

$$\rho_{sc}(\Lambda) = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} \mathrm{d}x \sqrt{2m(\Lambda - V(x))} \theta(\Lambda - V(x)) \tag{3.115}$$

The theta function reduces the integration over x to an integration between the turning points:

$$\rho_{sc}(\Lambda) = \frac{1}{\pi\hbar} \int_a^b \mathrm{d}x \sqrt{2m(\Lambda - V(x))} \tag{3.116}$$

$$= \frac{1}{\pi\hbar} \int_a^b \mathrm{d}x \; p(x), \tag{3.117}$$

where $p(x)$ is the momenta of the particle with energy Λ.

There is a nice interpretation of this formula in terms of classical phase space. A particle of energy less or equal to Λ verifies the inequality

$$\frac{p^2}{2m} + V(x) \leq \Lambda \tag{3.118}$$

The inequality above corresponds to a surface in the (x, p) plane, which is drawn in figure (3.9). In that plane, the turning points a and b are at $(a, 0)$ and $(b, 0)$ since the momentum vanishes at the turning points. These are on the boundary of the surface carved out by the inequality since $V(a) = V(b) = \Lambda$. We can therefore relate the area of this surface, $\Omega(\Lambda)$, to the integral in $\rho_{sc}(\Lambda)$ from equation (3.117):

$$\Omega(\Lambda) \equiv \text{area of phase space with } E < \Lambda = 2 \int_a^b p(x)\mathrm{d}x \tag{3.119}$$

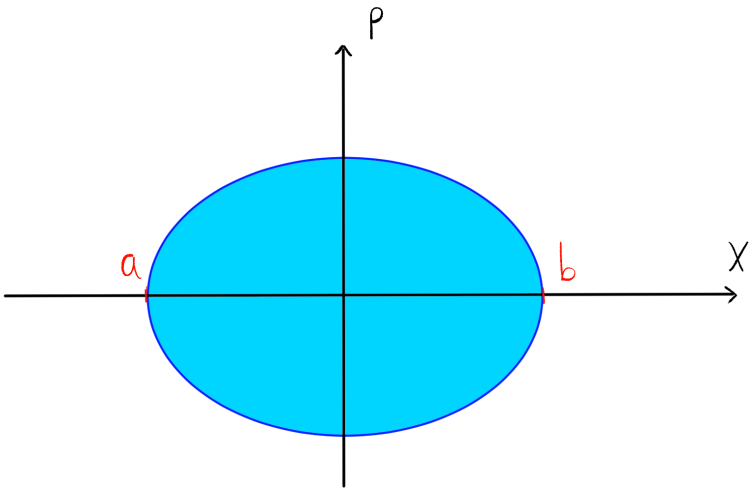


Figure 3.9: In light blue, the region described by the inequality (3.118). The turning points a and b are on the edge of the region.

Therefore, we have

$$\rho_{sc}(\Lambda) = \frac{\Omega(\Lambda)}{2\pi\hbar} \tag{3.120}$$

The exact spectral density counts the number of states with energy less than Λ, and therefore we have $\rho(E_n + \epsilon) = n + 1$ for a small ϵ (we start with the ground state energy E_0). In the semiclassical case, we are missing the feature of discrete jumps at each energy levels, and we instead have a smoothed out function that we can approximate as $\rho_{sc}(E_n) = n + \frac{1}{2}$. Expressing this equation in terms of phase space volume, we find the **Bohr-Sommerfeld quantization condition**

$$\Omega(E_n) = (n + 1/2)h, \tag{3.121}$$

which tells us that the unit volume of the classical phase space corresponding to a quantum state is equal to h. This semiclassical approximation is really only valid for large n, since for small n we are very sensitive to quantum effects.

Summary of Lecture 9

- Semiclassical fixed energy propagator, single saddle point:

$$K_{sc}(E; x_f, x_i) = \frac{1}{\sqrt{v_i v_f}} e^{\frac{i}{\hbar}\int_{x_i}^{x_f} \mathrm{d}x\, p(x)}$$

- Multiple saddle points (N_n = number of turning points):

$$K_{sc}(E; x_f, x_i) = \sum_n \frac{e^{-i\frac{\pi}{2}N_n}}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\int_{x_i}^{x_f} \mathrm{d}x_{(n)}\, p(x)}$$

- Semiclassical approximation to the transmission probability

$$P_{sc} = \exp\left(-\frac{2}{\hbar}\int_a^b \mathrm{d}z\, \sqrt{2m\left(V(z) - E\right)}\right)$$

- Semiclassical approximation to the spectral density:

$$\rho_{sc}(\Lambda) = \frac{\Omega(\Lambda)}{2\pi\hbar},$$

  where $\Omega(\Lambda)$ is the phase space volume with $E < \Lambda$, or in formulas $\Omega(\Lambda) = 2\int_a^b p(x)\mathrm{d}x$.

- Bohr-Sommerfeld quantization condition:

$$\Omega(E_n) = \left(n + \frac{1}{2}\right) h$$

Lecture 10 - Instantons

In quantum physics, perturbation theory can miss crucial effects. As a first example, let us look at the simple example of the metastable state.

Example 1: Metastable state
Consider the potential $V(x) = \frac{1}{2}m\omega^2x^2 + \lambda x^3$, where λ is small. For $\lambda = 0$, we know that the ground state with energy $E_0 = \frac{\hbar\omega}{2}$ is localized at $x = 0$. If we now set λ to be small but nonzero, there will be a probability of tunneling to the unbounded region at $x < 0$ (see figure 3.10), which means that the ground state becomes unstable.

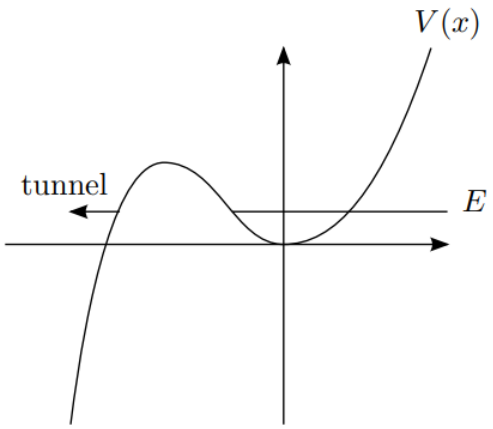


Figure 3.10: The ground state localized around the local minimum of $V(x)$ is unstable due to the nonzero tunneling probability.

If we consider perturbation theory in λ, we would find the following energy levels:

$$E_n = \hbar\omega(n + 1/2) + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \tag{3.122}$$

There will be no sign of the instability of the ground state. In order to explain this, recall the tunneling probability formula from last week:

$$P = \exp\left(-\frac{2}{\hbar}\int_a^b \mathrm{d}x\sqrt{2m(V(x) - E)}\right), \tag{3.123}$$

where a and b are the classical turning points. In order to see the dependency on λ, consider a particle with $E = 0$. Then, $V(x) = 0$ has two solutions:

$$x^2\left(\frac{1}{2}m\omega^2 + \lambda x\right) = 0 \implies x = 0,\ x = a \equiv -\frac{m\omega^2}{2\lambda} \tag{3.124}$$

Therefore, the tunneling probability is given by

$$P = \exp\left(-\frac{2}{\hbar}\int_a^0 \mathrm{d}x\sqrt{m^2\omega^2x^2 + 2m\lambda x^3}\right) \tag{3.125}$$

We would now like to take the perturbative limit $\lambda \to 0$. In order to compute the integral, we would naively remove the second term in the square root, but this is not correct. Indeed, as $\lambda \to 0$, $a \to -\infty$ and there is therefore a region of integration where $x \sim a$ is very large, meaning that both terms in the square root are actually of the same order. In fact, the integral can be computed exactly without taking any limits! To see this more clearly, we compute the integral by changing variables using $x = ay$ to have a dimensionless and tractable integral.

$$I \equiv \int_a^0 \mathrm{d}x \sqrt{m^2\omega^2 x^2 + 2m\lambda x^3} \tag{3.126}$$

$$= \frac{m^3\omega^5}{4\lambda^2} \int_0^1 \mathrm{d}y\, y\sqrt{1-y} \tag{3.127}$$

$$= \frac{m^3\omega^5}{4\lambda^2} \left(\int_0^1 \mathrm{d}z\, z^{1/2} - \int_0^1 \mathrm{d}z\, z^{3/2} \right) \quad (z = 1-y) \tag{3.128}$$

$$= \frac{m^3\omega^5}{15\lambda^2} \tag{3.129}$$

Therefore, the tunneling probability explicitly reads

$$P = \exp\left(-\frac{2}{\hbar} \frac{m^3\omega^5}{15\lambda^2} \right) \equiv \exp\left(-\frac{c}{\lambda^2} \right) \tag{3.130}$$

for some constant c.

In the limit $\lambda \to 0$, P goes to 0 **faster than any polynomial function of** λ! This is why the instability is **non-perturbative**: the effect is invisible in perturbation theory since it is smaller than any perturbative effect (λ^k).

Example 2: Double well potential

Consider the potential $V(x) = \frac{\lambda}{4!}(x^2 - a^2)^2$. In 1d quantum mechanics, there can be no degeneracies in energy levels, so we expect the first two energy levels to verify $E_1 > E_0$ (for a proof, see appendix B.1). In practice, the ground state wavefunction will not have zeros and the first excited wavefunction will have one zero. However, perturbation theory gives us a different picture. We expand the potential around the minima $x = a$:

$$V(a+y) = \frac{\lambda}{6}a^2y^2 + \frac{\lambda}{6}ay^3 + \frac{\lambda}{4!}y^4 \tag{3.131}$$

We can think of this as a regular harmonic oscillator with $\frac{1}{2}m\omega^2 = \frac{\lambda}{6}a^2$, with some cubic and quartic perturbation. For small λ, we can 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! By symmetry [4], the same can be done in the other minimum, which will find the same energy levels, but with wavefunctions localized around $-a$. If we consider the whole system in perturbation theory, we will see 2-fold degeneracy in the energy levels coming from the wavefunctions localized in either

[4] The expansion around the other minimum is done using $x = -a - y'$, but by reflection symmetry $V(-a-y') = V(a+y')$.

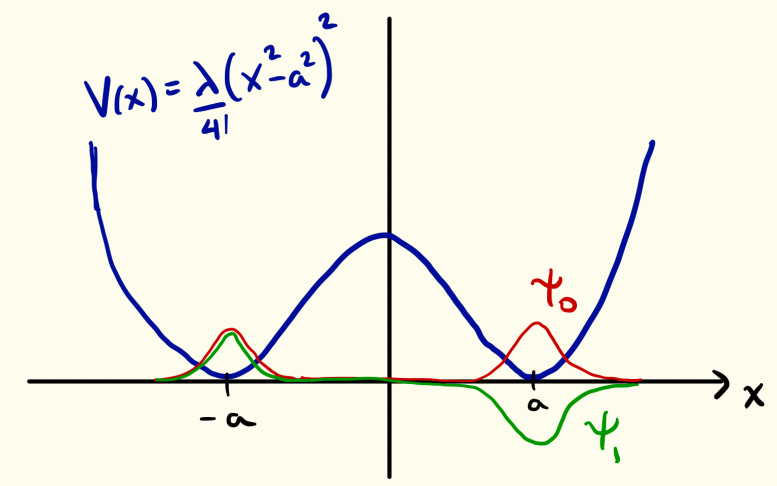


Figure 3.11: The double well potential with the first two energy eigenstate wavefunctions.

potential, which contradicts the initial statement $E_1 > E_0$! This problem is resolved by non-perturbative effects, which will save us and split the degeneracy.

Let us setup some notation. We define ω as

$$\omega = \sqrt{\frac{\lambda}{3m}}a \tag{3.132}$$

so that

$$V(a+y) = \frac{1}{2}m\omega^2 y^2 + \frac{1}{2}\omega\sqrt{\frac{m\lambda}{3}}y^3 + \frac{\lambda}{4!}y^4 \tag{3.133}$$

Now we clearly see the harmonic oscillator potential, and the perturbations: the cubic perturbation is proportional to $\lambda^{1/2}$ and the quartic is proportional to λ. The potential depends on two parameters: λ and a. Alternatively, we can express our results in terms of λ and ω which is sometimes more convenient.

In perturbation theory (in one of the wells),

$$E_n = \hbar\omega(n+1/2)\left(1 + \bar{\lambda}E_n^{(1)} + \bar{\lambda}^2 E_n^{(2)} + \dots\right) \tag{3.134}$$

where $\bar{\lambda}$ is the dimensionless expansion parameter,

$$\bar{\lambda} = \frac{\hbar\lambda}{m^2\omega^3}. \tag{3.135}$$

As explained previously, in perturbation theory there are two states for each energy level, localized at a and $-a$ respectively. The splitting $E_1 - E_0$ vanishes to all orders in $\bar{\lambda}$, but we will prove later that

$$E_1 - E_0 \propto e^{-\frac{2}{\bar{\lambda}}}, \tag{3.136}$$

which is a non-perturbative effect: it cannot be obtained by simple perturbation theory.

Instantons in the double well potential

We want to study in depth the ground state of the double well potential $V(x) = \frac{\lambda}{4!}(x^2 - a^2)^2$. To do so, we will go back to the Euclidean propagator:

$$K(x_f, x_i; \beta) = \langle x_f | \, e^{-\frac{\beta}{\hbar}H} \, | x_i \rangle \tag{3.137}$$

After inserting a basis of energy eigenstates, we find

$$K(x_f, x_i; \beta) = \sum_n e^{-\frac{\beta}{\hbar}E_n} \psi_n(x_f)\psi_n^*(x_i) = \int_{x(-\beta/2)=x_i}^{x(\beta/2)=x_f} \mathcal{D}[x] e^{-\frac{1}{\hbar}S_E[x]} \tag{3.138}$$

At large β, we will pick up the lowest energy states, and will therefore be able to see the splitting explicitly. In order to perform the computation, we will use the semiclassical approximation for the path integral.

The Euclidean action for the double well potential is given by

$$S_E = \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \; \frac{1}{2} m\dot{x}^2 + \frac{\lambda}{4!}(x^2 - a^2)^2 \tag{3.139}$$

In order to make the dependencies on the different parameters more explicit, consider $\tau = c\eta$, $x = aq$:

$$S_E = \int_{-\frac{\beta}{2c}}^{\frac{\beta}{2c}} \mathrm{d}\eta \; \left(\frac{ma^2}{c} \frac{1}{2} \dot{q}^2 + \frac{\lambda a^4 c}{4!}(q^2 - 1)^2 \right). \tag{3.140}$$

Now we want to choose the constant c so that both terms in parenthesis have the same prefactor:

$$\frac{ma^2}{c} = \lambda a^4 c \implies c = \sqrt{\frac{m}{\lambda a^2}} = \frac{1}{\sqrt{3}\omega} \tag{3.141}$$

we therefore end up with

$$S_E = a^3 \sqrt{m\lambda} \int_{-\frac{\sqrt{3}\beta\omega}{2}}^{\frac{\sqrt{3}\beta\omega}{2}} \mathrm{d}\eta \; \left(\frac{1}{2}\dot{q}^2 + \frac{1}{4!}(q^2 - 1)^2 \right). \tag{3.142}$$

Now the integral is an $\mathcal{O}(1)$ dimensionless number, and therefore the semiclassical approximation is

$$1 \ll \frac{S_E}{\hbar} = \frac{a^3\sqrt{m\lambda}}{\hbar} \tag{3.143}$$

We reformulate this condition in terms of $\bar{\lambda}$ (see eqs. 3.132 and 3.135):

$$1 \ll \frac{a^3\sqrt{m\lambda}}{\hbar} = \frac{3^{3/2}}{\bar{\lambda}} \Leftrightarrow \bar{\lambda} \ll 1 \tag{3.144}$$

As expected, **the semiclassical approximation is justified when $\bar{\lambda}$ is small, which is the same requirement as regular perturbation theory**. However, the resulting effects are much smaller than perturbation theory since we are considering $e^{-\frac{S_E}{\hbar}} \sim e^{-\frac{1}{\lambda}}$ in the path integral.

Let us now do the saddle point approximation of the path integral.

$$K(x_f, x_i; \beta) = \int_{x(-\beta/2)=x_i}^{x(\beta/2)=x_f} \mathcal{D}[x] e^{-\frac{1}{\hbar} S_E[x]} \tag{3.145}$$

$$= \sum_k I_k e^{-\frac{1}{\hbar} S_E[x_k]} \tag{3.146}$$

where k labels the saddle points, and I_k is some prefactor which we will consider later. The saddle points are **paths** $x_k(\tau)$ on which the Euclidean action is stationary, i.e.

$$\left.\frac{\delta S_E}{\delta x}\right|_{x=x_k} = 0 \Leftrightarrow m\ddot{x}_k = V'(x_k) \quad \text{(Euclidean equation of motion)} \tag{3.147}$$

Note now that the Euclidean equation of motion above corresponds to the real time equation of motion with a reversed potential $V_E(x) = -V(x)$ (see figure 3.12), which will allow us to use our physical intuition to find the saddle points.

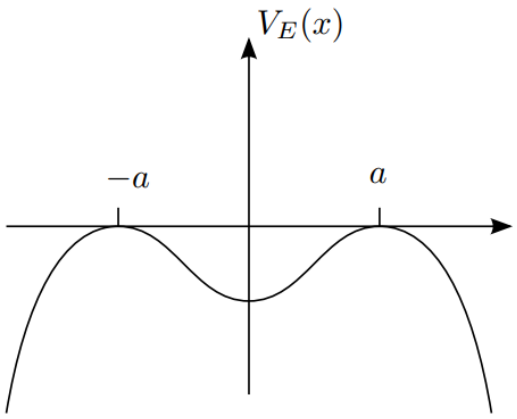


Figure 3.12: Saddle points of the Euclidean path integral can be interpreted as classical trajectories in the inverted potential $V_E(x) = -V(x)$.

Until now we have been general in our choice of x_i and x_f. However, we will now focus on the special cases of $x_i = \pm a$ and $x_f = \pm a$, since those will be the easiest to compute. By symmetry,

$$K(a, a; \beta) = \langle a | \, e^{-\frac{\beta}{\hbar} H} \, | a \rangle = \langle -a | \, e^{-\frac{\beta}{\hbar} H} \, | -a \rangle \tag{3.148}$$

$$K(a, -a; \beta) = \langle a | \, e^{-\frac{\beta}{\hbar} H} \, | -a \rangle = \langle -a | \, e^{-\frac{\beta}{\hbar} H} \, | a \rangle \tag{3.149}$$

As said previously, we will look at the large β limit to study the lowest energy states. The potential admits the trivial solutions $x(\tau) = \pm a$ (staying at the top of either hills), which will be the leading contribution to the $a \to a$ and the $-a \to -a$ propagators.

However, there are also nontrivial solutions, which are called **instantons**. The instanton is a solution which starts at $x = -a$ at $\tau = -\infty$ (this solution will be exact in the $\beta \to \infty$ limit since we want the boundary conditions to be at $\tau = \pm\infty$), rolls down the hill and reaches $x = a$ at $\tau = +\infty$. The **anti-instanton** does the opposite: it goes from a at $\tau = -\infty$ to $-a$ at $\tau = +\infty$. These trajectories both have Euclidean energy $E_E = \frac{1}{2}m\dot{x}^2 + V_E(x) = 0$, as they start with zero velocity at $x = \pm a$ and arrive at $x = \mp a$ with zero velocity. Therefore, we can be more quantitative and arrive at the expression:

$$\frac{1}{2}m\dot{x}^2 - V(x) = 0 \implies \dot{x} = \pm\sqrt{\frac{2V(x)}{m}}, \tag{3.150}$$

where the $\pm$ sign corresponds to the instanton and anti-instanton. We can then compute the Euclidean action for the instanton S_I:

$$S_I = \int_{-\infty}^{\infty} \mathrm{d}\tau \ \frac{1}{2}m\dot{x}^2 + V(x) = \int_{-\infty}^{\infty} \mathrm{d}\tau \ m\dot{x}^2 - E_E \tag{3.151}$$

$$= \int_{-a}^{a} \mathrm{d}x \ \sqrt{2mV(x)} \tag{3.152}$$

Note that the anti-instanton action is exactly the same: $S_I = S_A$.

In the case of the double well potential $V(x) = \frac{\lambda}{4!}(x^2 - a^2)^2$, we can find the instanton trajectory $x_I(\tau)$ explicitly:

$$\dot{x}_I(\tau) = +\sqrt{\frac{\lambda}{12m}}(a^2 - x_I^2(\tau)) \tag{3.153}$$

$$\implies x(\tau) = a\tanh\left(\frac{\omega}{2}(\tau - \tau_0)\right) \tag{3.154}$$

where in the first line we used $\sqrt{(x^2 - a^2)^2} = a^2 - x^2$ since the instanton is always between the two hills ($-a \le x \le a$), and τ_0 is just an integration constant. This reflects the time-translation invariance of the problem: the instanton goes from $-a$ to a at $\tau \approx \tau_0$, which is arbitrary. The trajectory is presented in figure 3.13.

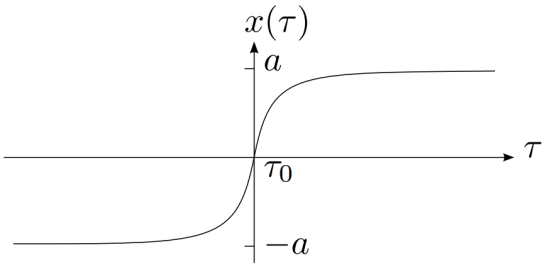


Figure 3.13: The double-well potential instanton trajectory in the $\beta \to \infty$ limit.

The instanton action can also be explicitly computed:

$$\frac{S_I}{\hbar} = \frac{1}{\hbar}\int_{-a}^{a} \mathrm{d}x\, \sqrt{\frac{m\lambda}{12}}(a^2 - x^2) \tag{3.155}$$

$$= \frac{2}{\frac{=}{\lambda}} \tag{3.156}$$

Therefore, the saddle point approximation exhibits the nonperturbative effect:

$$e^{-\frac{S_I}{\hbar}} = e^{-\frac{2}{\lambda}} \tag{3.157}$$

Note now that since we are taking the $\beta \to \infty$ limit, we are working on time scales that are much larger than $\frac{1}{\omega}$ (the only parameter in the problem with units of time). Now in the $|\tau - \tau_0| \gg \frac{1}{\omega}$ limit, we expect to be very close to $\pm a$ and indeed,

$$\left|x_I^2(\tau) - a^2\right| = a^2 \frac{1}{\cosh^2\left(\frac{\omega}{2}(\tau - \tau_0)\right)} \tag{3.158}$$

$$\xrightarrow{\omega|\tau-\tau_0|\gg 1} a^2 e^{-\omega|\tau-\tau_0|} \tag{3.159}$$

We are therefore exponentially close to a (or $-a$ in the past) at time scales much bigger than $\frac{1}{\omega}$. For this reason, our trajectory really looks like a step function. In a sense, since we are considering large time scales, we are looking at a "zoomed-out" version of figure 3.13. This is where the name **instanton** comes from: they exist for a very brief period of time $\Delta\tau \sim \frac{1}{\omega}$.

Because instantons go from $-a$ to a in such a short time, we should also consider **multi-instanton** solutions to the Euclidean equations of motion[5]. It is possible to have a solution going from $-a$ to a at a time τ_1, then back to $-a$ at τ_2, and finally back to a at τ_3.

Let us setup the notation: we label by I the instantons (going from $-a$ to a) and by A the anti-instantons (from a to $-a$). We have

$$x_I(\tau) = af(\tau - \tau_1) \tag{3.160}$$

$$x_A(\tau) = af(\tau_2 - \tau), \tag{3.161}$$

where f is a function interpolating from -1 to 1 in general (for the double well, we found $f(\tau) = \tanh(\omega\tau/2)$) and τ_1 and τ_2 are for now arbitrary times at which the instanton/anti-instanton exist. Then, we can define

$$x_{IA}(\tau) = af(\tau - \tau_1)f(\tau_2 - \tau), \tag{3.162}$$

with $\tau_1 < \tau_2$. This is only an approximate solution to the Euclidean EOM

$$\frac{\delta S_E}{\delta x} = m\ddot{x} - V'(x) = 0, \tag{3.163}$$

[5]Note that these are only approximate solutions.

although a very good one. Indeed, it can be shown that [6]

$$\left.\frac{\delta S_E}{\delta x}\right|_{x=x_{IA}} \sim ma\omega^2 e^{-\omega|\tau_1-\tau_2|} \tag{3.164}$$

Therefore, if the instanton and anti-instanton are well-separated ($|\tau_1 - \tau_2| \gg \frac{1}{\omega}$), x_{IA} is an approximate solution of the Euclidean EOM. In fact, we shall see that

$$\omega|\tau_1 - \tau_2| \sim e^{\frac{S_I}{\hbar}} \gg 1, \tag{3.165}$$

so the error we are making is **doubly exponentially small**:

$$\left.\frac{\delta S_E}{\delta x}\right|_{x=x_{IA}} \sim ma\omega^2 \exp\left(-e^{\frac{S_I}{\hbar}}\right) \tag{3.166}$$

As long as we only need to consider situations where 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. In other words, we know that we are making a small error when considering x_{IA} as a solution, but since this error is smaller than other effects we have previously neglected, we should still consider x_{IA} as an important saddle point.

Dilute instanton gas approximation

In this section we will assemble the pieces to compute the saddle point approximation propagator. As explained above, we will need to sum the contributions from many classical paths made of instanton and anti-instantons appearing at different euclidean times.

Consider the propagator from $-a$ to a. We need to sum the contribution from the single instanton, and the contributions from going back and forth with instantons and anti-instantons. Schematically,

$$\langle a|\, e^{-\frac{\beta}{\hbar}H}\, |-a\rangle = \#e^{-\frac{S_I}{\hbar}} + \#e^{-\frac{S_{IAI}}{\hbar}} + \dots \tag{3.167}$$

Similarly, for a to a, we need to compute

$$\langle a|\, e^{-\frac{\beta}{\hbar}H}\, |a\rangle = \#e^{-\frac{S_{AI}}{\hbar}} + \#e^{-\frac{S_{AIAI}}{\hbar}} + \dots \tag{3.168}$$

Let's go step by step:

- **Action:** a given saddle point has in general N_I instantons and N_A anti-instantons. Since $S_I = S_A$, the action for such a trajectory is $S = NS_I$[7], with $N = N_I + N_A$.

[6] To see this notice that $f(z) \approx \pm(1 - e^{-\omega|z|})$ for $\omega|z| \gg 1$. If we assume $\omega|\tau_1 - \tau_2| \gg 1$ then for any τ we can use this approximation for at least one of the functions f in (3.162).

[7] Since the action is just the integral over time, we can split it into different regions corresponding to each instanton and anti-instanton, which is why the action "factorizes".

Now normally in the saddle-point approximation, the "lowest" point gives the biggest contribution, but here we are considering "large" saddle points when N is large. The reason we must keep those larger saddle points which naively contribute **less** is because of some other contribution discussed below (the **sum over kink locations**), which enhances the large N saddle points by a factor β^N. In the very large β limit, the multi-instanton saddle points with $S = NS_I$ are therefore important!

- **Prefactor:** recall that the prefactor was given by

$$\text{prefactor } = \tilde{\mathcal{N}} \det \left(\frac{\delta^2 S}{\delta x^2} \right)^{-1/2} \tag{3.169}$$

It is straightforward to show that

$$\frac{\delta^2 S}{\delta x^2} = -m \frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + V''(x) \tag{3.170}$$

Note now that most of the time, $x(\tau) = \pm a$, so we can approximate $V''(x) \approx V''(\pm a) = m\omega^2$, which is the harmonic oscillator. Therefore, "most of the time", the prefactor is the same as the one for the harmonic oscillator. This prefactor, in the limit $\omega\beta \to \infty$, can be easily extracted from the Euclidean harmonic oscillator propagator (eq. 2.17):

$$\text{HO prefactor } = \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} e^{-\frac{\omega\beta}{2}} \tag{3.171}$$

However, we know that this is just an approximation. In order to account for our error, we introduce some factor R for each instanton and anti-instanton:

$$\text{prefactor } = \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} e^{-\frac{\omega\beta}{2}} R^N, \quad (N = N_I + N_A) \tag{3.172}$$

In other words, for every "jump", there is an additional factor R. Finding the expression for R is very time-consuming and is not necessary for our discussion, but the computation is done in the appendix (B.5). Again, the reason why R is the same for each jump comes from the factorization property of the propagator: going from x to y is the same as going from x to z and from z to y, so we can isolate the contribution from each jump.

- **Sum over kink locations:** each trajectory is characterized by the number of instantons N_I and anti-instantons N_A, but also by the times τ_k, $k = 1, \ldots, N$ at which the jumps happen. In order to sum over all trajectories, we must multiply by a factor corresponding to these possibilities[8]. We call this factor M, and it is given by

$$M = \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_N \int_{-\beta/2}^{\tau_N} \mathrm{d}\tau_{N_1} \ldots \int_{-\beta/2}^{\tau_2} \mathrm{d}\tau_1 = \frac{\beta^N}{N!} \tag{3.173}$$

[8]Because of time-translation invariance, the exact times τ_k do not affect other parts of the overall computation. However, an overall multiplicative factor needs to be included to account for the large (infinite) number of possible trajectories

Note the integration bounds specified above to respect the ordering $\tau_N > \ldots > \tau_1$. The value of M can be obtained by computing the integrals explicitly, or simply by computing the overall volume without the ordering, giving the β^N factor, and then dividing by $N!$ to select the proper ordering.

- **Instanton/anti-instanton ordering:** this contribution is trivial for the double-well potential, but it becomes relevant for more general potentials. Since we are only allowed to go from a to $-a$ and vice-versa, all our trajectories alternate between instanton and anti-instanton. However, in general, one might have to compute the multiplicity coming from different trajectories with the same N_I and N_A. For example, in the triple well potential (3 hills at $-a$, 0 and a), the trajectories $IAIA$ and $IIAA$ are both relevant to go from $-a$ to a, and we would need to account for this multiplicity. In our computation however, this is not important, since for a given $N = N_I + N_A$, there is only one allowed configuration of I's and A's.

Now that we have all the pieces, we can compute:

$$\langle a| e^{-\frac{\beta}{\hbar}H} |-a\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{\omega\beta}{2}} \sum_{N\text{odd}} \frac{1}{N!} \left(\beta R e^{-\frac{S_I}{\hbar}}\right)^N \tag{3.174}$$

$$\langle a| e^{-\frac{\beta}{\hbar}H} |a\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{\omega\beta}{2}} \sum_{N\text{even}} \frac{1}{N!} \left(\beta R e^{-\frac{S_I}{\hbar}}\right)^N \tag{3.175}$$

Therefore, we have the final result for both propagators:

$$\langle a| e^{-\frac{\beta}{\hbar}H} |\pm a\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{\omega\beta}{2}} \frac{1}{2} \left(e^{\beta R e^{-\frac{S_I}{\hbar}}} \pm e^{-\beta R e^{-\frac{S_I}{\hbar}}}\right) \tag{3.176}$$

This allows us to extract the energy levels! Indeed, we know (eq. 3.138) that

$$\langle a| e^{-\frac{\beta}{\hbar}H} |\pm a\rangle = \sum_n e^{-\frac{\beta}{\hbar}E_n} \psi_n(a)\psi_n^*(\pm a), \tag{3.177}$$

and therefore we can extract the energy levels from equation (3.176) by looking at the exponentials (they are the only place where β appears). The first two energy levels are:

$$E_0 = \frac{\hbar\omega}{2} - \hbar R e^{-S_I/\hbar} \tag{3.178}$$

$$E_1 = \frac{\hbar\omega}{2} + \hbar R e^{-S_I/\hbar}. \tag{3.179}$$

The **energy splitting is non-perturbative** as expected:

$$E_1 - E_0 = 2\hbar R e^{-\frac{2}{\lambda}} \tag{3.180}$$

Furthermore, we can directly extract

$$|\psi_0(a)|^2 = \psi_0(a)\psi_0^*(a) = \frac{1}{2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \tag{3.181}$$

$$|\psi_1(a)|^2 = \psi_1(a)\psi_1^*(a) = \frac{1}{2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \tag{3.182}$$

from $\langle a| e^{-\frac{\beta}{\hbar}H} |a\rangle$. The fact that the ground state wavefunction has zero nodes (ψ_0 is even $\psi_0(a) = \psi_0(-a)$) and the first excited state has one node (ψ_1 is odd) can also be seen from the $\pm$ sign in front of the second exponential in parenthesis in equation (3.176). All of the above comments are compatible with the idea that the ground state and first excited state of the double well potential are in fact even and odd linear combinations of harmonic oscillator ground states in each well:

$$\psi_0^{(\mathrm{DW})}(x) = \frac{1}{\sqrt{2}}\left(\psi_0^{\mathrm{HO}}(x+a) + \psi_0^{\mathrm{HO}}(x-a)\right) \tag{3.183}$$

$$\psi_1^{(\mathrm{DW})}(x) = \frac{1}{\sqrt{2}}\left(\psi_0^{\mathrm{HO}}(x+a) - \psi_0^{\mathrm{HO}}(x-a)\right) \tag{3.184}$$

Remarks:

- **Perturbative corrections:** in our derivation, we neglected the perturbative corrections. Schematically, we have done a saddle point approximation where $e^{-S_I/\hbar}$ led to the $e^{-\frac{2}{\lambda}}$ term, the quadratic order led to the prefactor, and we dropped any higher order $\frac{\delta^k S}{\delta x^k}$. These higher order terms are actually just the usual perturbation theory from chapter 2, which we compute using Feynman diagrams. In practice, since the instantons spend most of the time at the minima $\pm a$, we can simply do the usual perturbation theory computation in the anharmonic potential (eq. 3.133).

  For this reason, equations (3.178) and (3.179) are wrong! We wrote the nonperturbative effects due to $e^{-\frac{2}{\lambda}}$, but not the much bigger perturbative effects. We should have written

  $$E_0 = \frac{\hbar\omega}{2}(1 + \mathcal{O}(\bar{\lambda}) + \ldots) - \hbar R e^{-S_I/\hbar}(1 + \mathcal{O}(\bar{\lambda}) + \ldots) \tag{3.185}$$

  $$E_1 = \frac{\hbar\omega}{2}(1 + \mathcal{O}(\bar{\lambda}) + \ldots) + \hbar R e^{-S_I/\hbar}(1 + \mathcal{O}(\bar{\lambda}) + \ldots). \tag{3.186}$$

  The important punchline is that these perturbative corrections are the **same** for E_0 and E_1, which is why the splitting $E_1 - E_0$ vanishes when considering only perturbation theory!

- **Validity of the dilute instanton gas approximation:**
  Recall that we used sums of the type

  $$\sum_N \frac{1}{N!}\left(\beta R e^{-S_I/\hbar}\right)^N \tag{3.187}$$

  Each term in the sum contributes a different value to the final result, but you can convince yourself that the dominant contribution comes from the terms near $N \sim \beta R e^{-S_I/\hbar}$. This is a useful tool to estimate the typical time separation $\Delta\tau$ between instantons. Assuming they are uniformly distributed, we see that

  $$\Delta\tau = \frac{\beta}{N} \sim \frac{1}{R} e^{\frac{S_I}{\hbar}} \tag{3.188}$$

This justifies our assumption from equation (3.165).

In order for the dilute instanton gas approximation to be valid, the time separation between instantons should be much larger than the instanton duration $\frac{1}{\omega}$, i.e.

$$\frac{\beta}{N} \sim \frac{1}{R} e^{\frac{S_I}{\hbar}} \gg \frac{1}{\omega}. \tag{3.189}$$

This is automatically verified since we assumed $\frac{S_I}{\hbar} \gg 1$ to do the semiclassical approximation.

- **Avoiding multi-instantons:**
  Consider the following range of values of β:

$$\frac{1}{\omega} \ll \beta \ll \frac{1}{R} e^{S_I/\hbar} \tag{3.190}$$

The first requirement $\frac{1}{\omega} \ll \beta$ is present to project onto the lowest energy states. We can think of $\hat{H}$ as a 2×2 matrix acting on the subspace $\{|a\rangle, |-a\rangle\}$. Then, consider the matrix elements (3.174) and (3.175), but since $\beta \ll \frac{1}{R} e^{S_I/\hbar}$ we only keep the leading term in each sum:

$$\langle a| e^{-\frac{\beta}{\hbar}\hat{H}} |-a\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{\omega\beta}{2}} \left(\beta R e^{-\frac{S_I}{\hbar}}\right) + \dots \tag{3.191}$$

$$\langle a| e^{-\frac{\beta}{\hbar}\hat{H}} |a\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{\omega\beta}{2}} + \dots \tag{3.192}$$

where the $\dots$ symbolize perturbative corrections as explained earlier. Then we can write[9]

$$e^{-\frac{\beta}{\hbar}\hat{H}} = e^{-\frac{\omega\beta}{2}} \begin{pmatrix} 1+\dots & \beta R e^{-\frac{S_I}{\hbar}} + \dots \\ \beta R e^{-\frac{S_I}{\hbar}} + \dots & 1+\dots \end{pmatrix} \tag{3.193}$$

Again, because of the assumption $\beta \ll \frac{1}{R} e^{S_I/\hbar}$, we can exponentiate the matrix!

$$e^{-\frac{\beta}{\hbar}\hat{H}} \approx \exp\left[-\frac{\beta}{\hbar}\left(\frac{\omega\hbar}{2}(1+\mathcal{O}(\bar{\lambda}))\begin{pmatrix}1&0\\0&1\end{pmatrix} + \hbar R e^{-\frac{S_I}{\hbar}}(1+\mathcal{O}(\bar{\lambda}))\begin{pmatrix}0&1\\1&0\end{pmatrix}\right)\right] \tag{3.194}$$

We can then read off the **effective Hamiltonian** $\hat{H}_{\text{eff}}$ on the 2-level subspace:

$$\hat{H}_{\text{eff}} = \frac{\omega\hbar}{2}(1+\mathcal{O}(\bar{\lambda}))\begin{pmatrix}1&0\\0&1\end{pmatrix} + \hbar R e^{-\frac{S_I}{\hbar}}(1+\mathcal{O}(\bar{\lambda}))\begin{pmatrix}0&1\\1&0\end{pmatrix} \tag{3.195}$$

It is straightforward to find the 2 eigenvalues of $\hat{H}_{\text{eff}}$, E_0 and E_1, and to see that

$$E_1 - E_0 = 2\hbar R e^{-S_I/\hbar}, \tag{3.196}$$

[9]The overall factor $\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}$ can simply be included in the definitions of $|\pm a\rangle$ and is irrelevant for this discussion.

which is what we had obtained earlier by summing contributions from multi-instanton trajectories. Using this result, we can reformulate our initial assumption on β (eq. 3.190) as

$$\beta\omega \gg 1 \quad \text{and} \quad \frac{\beta}{\hbar}(E_1 - E_0) \ll 1 \tag{3.197}$$

As a last comment, there is a simple intuition behind the choice $\beta \ll \frac{1}{R}e^{S_I/\hbar}$: since we argued $\frac{1}{R}e^{S_I/\hbar}$ is the typical time separation between different instantons, the requirement $\beta \ll \frac{1}{R}e^{S_I/\hbar}$ means that we only have time for one instanton, which corresponds to the simplifications made above.

In appendix B.5 we compute the instanton pre-factor. This leads to the final formula:

$$\boxed{E_1 - E_0 \approx 2\hbar\omega e^{-\frac{1}{\hbar}S_I}\left(\frac{m\omega a^2}{\pi\hbar}\right)^{1/2}\exp\left(-\int_0^a \mathrm{d}x\left[\frac{1}{a-x} - \sqrt{\frac{m\omega^2}{2V(x)}}\right]\right)} \tag{3.198}$$

For the case $V(x) = \frac{\lambda}{4!}(x^2 - a^2)^2$, with $\frac{\lambda a^2}{3} = m\omega^2$, the last integral reads

$$I \equiv \int_0^a \mathrm{d}x\left[\frac{1}{a-x} - \sqrt{\frac{m\omega^2}{2V(x)}}\right] \tag{3.199}$$

$$= \int_0^a \mathrm{d}x\left[\frac{1}{a-x} - \frac{2a}{a^2-x^2}\right] = -\ln(2) \tag{3.200}$$

which implies

$$\boxed{E_1 - E_0 = 4\hbar\omega\sqrt{\frac{3}{\pi\bar{\lambda}}}e^{-\frac{2}{\bar{\lambda}}}}, \tag{3.201}$$

where $\bar{\lambda}$ is the dimensionless coupling defined in (3.135).

Summary of Lecture 10

- Particle in the double-well potential

$$V(x) = \lambda(x^2 - a^2)^2$$

has non-degenerate energy levels, so $E_1 - E_0 > 0$.

- Computation in dilute instanton gas approximation:

$$E_1 - E_0 \approx 2\hbar R e^{-\frac{S_I}{\hbar}} = 2\hbar R e^{-\frac{2}{\lambda}} \approx,$$

where R is a prefactor coming from the saddle point approximation (schematically $\sim \det \frac{\delta^2 S}{\delta x^2}$). This is a **non-perturbative** energy splitting.

- Single instanton dominates for

$$\text{width of instanton } = \frac{1}{\omega} \ll \beta \ll \frac{1}{R} e^{\frac{S_I}{\hbar}} = \text{ typical separation between instantons}$$

Equivalently,

$$\beta\omega \gg 1 \quad \text{and} \quad \frac{\beta}{\hbar}(E_1 - E_0) \ll 1$$

- The final formula (for $V(x) = V(-x)$) is

$$E_1 - E_0 \approx 2\hbar\omega e^{-\frac{1}{\hbar}S_I} \left(\frac{m\omega a^2}{\pi\hbar}\right)^{1/2} \exp\left(-\int_0^a \mathrm{d}x \left[\frac{1}{a-x} - \sqrt{\frac{m\omega^2}{2V(x)}}\right]\right)$$

Chapter 4

Interaction with an external electromagnetic field

Lecture 11 - Quantum particle in an EM field

Classical physics

Let us begin with a quick review of classical physics. The Minkowski metric is given by

$$\mathrm{d}s^2 = c^2\mathrm{d}t^2 - \mathrm{d}\mathbf{x}^2 = c^2\mathrm{d}\tau^2, \tag{4.1}$$

where τ is the proper time. The action for a relativistic point particle on a trajectory γ is

$$S = -mc^2 \int_\gamma \mathrm{d}\tau = -mc^2 \int_\gamma \mathrm{d}t \sqrt{1 - \frac{\dot{x}^2}{c^2}}. \tag{4.2}$$

Now consider an external electromagnetic field which can be described using the 4-potential $A_\mu = (\Phi, -c\mathbf{A})$. The action can now be written (using $x^\mu = (ct, \mathbf{x})$)

$$S = -mc^2 \int_\gamma \mathrm{d}\tau - \frac{e}{c} \int_\gamma A_\mu \mathrm{d}x^\mu \tag{4.3}$$

$$= -\int_\gamma \mathrm{d}t \left[mc^2 \sqrt{1 - \frac{\dot{\mathbf{x}}^2}{c^2}} + e\Phi - e\mathbf{A}\cdot\dot{\mathbf{x}} \right], \tag{4.4}$$

where e is the charge of the particle.

Electromagnetism is invariant under **gauge transformations** $A_\mu \to A_\mu + c\partial_\mu \alpha$, where α is an arbitrary function of spacetime. Under a gauge transformation, the action above changes by a boundary term:

$$S \to S - e(\alpha(\mathbf{x_f}, t_f) - \alpha(\mathbf{x_i}, t_i)), \tag{4.5}$$

where $(\mathbf{x_f}, t_f)$ and $(\mathbf{x_i}, t_i)$ are the endpoints of the trajectory γ. However, the equations of motion are unaffected! In fact, the equations of motion only depend on a local gauge invariant function of A_μ: $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$.

The conjugate momentum is given by

$$\mathbf{p} = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{x}}} = \frac{m\dot{\mathbf{x}}}{\sqrt{1 - \frac{\dot{\mathbf{x}}^2}{c^2}}} + e\mathbf{A} \tag{4.6}$$

Exercise 4.1 (Hamiltonian of charged particle in EM field)**.** *Show that the Hamiltonian of the particle is given by*

$$H = \mathbf{p} \cdot \dot{\mathbf{x}} - \mathcal{L} = \sqrt{(\mathbf{p} - e\mathbf{A})^2 c^2 + m^2 c^4} + e\Phi \tag{4.7}$$

How do gauge transformations affect $\mathbf{p}$ and H? Recall that under gauge transformations, the components of the 4-potential transform as:

$$\phi \xrightarrow{\text{G.T.}} \phi + \partial_t \alpha \tag{4.8}$$

$$\mathbf{A} \xrightarrow{\text{G.T.}} \mathbf{A} - \nabla \alpha \tag{4.9}$$

Therefore, we can extract the gauge transformation properties of the momentum and the hamiltonian from their definitions (eq. 4.6 and 4.7):

$$\mathbf{p} \xrightarrow{\text{G.T.}} \mathbf{p} - e\nabla \alpha \tag{4.10}$$

$$H \xrightarrow{\text{G.T.}} H + e\partial_t \alpha. \tag{4.11}$$

The momentum and hamiltonian are therefore **not** gauge invariant! The above is instead an example of a canonical transformation (which preserve the Poisson brackets). In other words, the **gauge transformation** of the electromagnetic 4-potential A_μ corresponds to a **canonical transformation** of the hamiltonian variables:

$$A_\mu \xrightarrow{\text{G.T.}} A_\mu + c\partial_\mu \alpha \tag{4.12}$$

$$\begin{cases} x^i \\ p^i \\ H \end{cases} \xrightarrow{\text{C.T.}} \begin{cases} x^i \\ p^i - e\partial_i \alpha \\ H + e\partial_t \alpha \end{cases} \tag{4.13}$$

Moreover, we can define a gauge invariant quantity, the **kinetic momentum $\mathbf{\Pi}$**, as

$$\mathbf{\Pi} = \mathbf{p} - e\mathbf{A} \tag{4.14}$$

Using equation (4.6), one can see that in the nonrelativistic limit, $\mathbf{\Pi} = m\dot{\mathbf{x}}$, i.e. it is related to the velocity of the particle.

Let us now move on to quantum physics.

Quantum physics

We have seen in equation (4.5) that the action changes by a boundary term under a gauge transformation. Therefore, the propagator changes by a phase:

$$K(x_f,t_f;x_i,t_i) = \int \mathcal{D}[x] e^{\frac{i}{\hbar}S} \tag{4.15}$$

$$\implies K(x_f,t_f;x_i,t_i) \xrightarrow{G.T.} K(x_f,t_f;x_i,t_i) e^{-\frac{ie}{\hbar}(\alpha(x_f,t_f)-\alpha(x_i,t_i))} \tag{4.16}$$

Now recall as well that

$$\psi(x_f,t_f) = \int_{-\infty}^{\infty} \mathrm{d}t_i \; K(x_f,t_f;x_i,t_i)\psi(x_i,t_i). \tag{4.17}$$

In order for the above equation to be gauge invariant, the wavefunction must transform as well, according to

$$\boxed{\psi(x,t) \xrightarrow{\text{G.T.}} e^{-\frac{ie}{\hbar}\alpha(x,t)}\psi(x,t)} \tag{4.18}$$

The quantum mechanical analogy of canonical transformations are unitary transformations $\psi \to U\psi$, with $U^\dagger U = UU^\dagger = 1$. Indeed, matrix elements of operators transform as

$$\langle\psi_1|\,\hat{O}\,|\psi_2\rangle \xrightarrow{\text{U.T.}} \langle\psi_1|\,\hat{U}^\dagger\hat{O}\hat{U}\,|\psi_2\rangle\,. \tag{4.19}$$

Similarly to the Heisenberg picture, one can say that unitary transformations leave the states invariant but transform operators as $\hat{O} \to \hat{U}^\dagger\hat{O}\hat{U}$. This transformation leaves commutation relations invariant, which is the definition of a canonical transformation:

$$[\hat{x},\hat{p}] = i\hbar \xrightarrow{\text{U.T.}} [\hat{U}^\dagger\hat{x}\hat{U},\hat{U}^\dagger\hat{p}\hat{U}] = \hat{U}^\dagger[\hat{x},\hat{p}]\hat{U} = i\hbar \tag{4.20}$$

To summarize, the gauge transformation of the wavefunction is an example of a unitary transformation, which is the quantum version of a canonical transformation in classical physics.

We would now like to take the **non-relativistic limit** ($\dot{x} \ll c$) of the Hamiltonian:

$$H_{\text{non-rel}} = mc^2 + \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\Phi. \tag{4.21}$$

Note that the constant mc^2 has no physical consequences, so we drop it from now on. After quantization, the Hamiltonian can be written as

$$\boxed{\hat{H} \equiv \frac{1}{2m}(\hat{\mathbf{p}} - e\mathbf{A}(\hat{\mathbf{x}}))^2 + e\Phi(\hat{\mathbf{x}})}\,. \tag{4.22}$$

Now we would like to see how the matrix element of $\hat{\mathbf{p}}$ transform under a gauge transformation. Using (eq. 4.18), we have

$$\langle\psi_1|\,\hat{\mathbf{p}}\,|\psi_2\rangle = \int \mathrm{d}^3x\, \psi_1^*(\mathbf{x})(-i\hbar\nabla)\psi_2(\mathbf{x}) \tag{4.23}$$

$$\xrightarrow{\text{G.T.}} \int \mathrm{d}^3x\, \psi_1^*(\mathbf{x}) e^{\frac{ie}{\hbar}\alpha}(-i\hbar\nabla)e^{-\frac{ie}{\hbar}\alpha}\psi_2(\mathbf{x}) \tag{4.24}$$

$$= \langle\psi_1|\,\hat{\mathbf{p}}\,|\psi_2\rangle - e\,\langle\psi_1|\,\nabla\alpha\,|\psi_2\rangle \tag{4.25}$$

However, the matrix elements of the **kinetic momentum operator** are gauge invariant:

$$\langle\psi_1|\,\hat{\mathbf{\Pi}}\,|\psi_2\rangle = \int \mathrm{d}^3x\,\psi_1^*(\mathbf{x})(-i\hbar\nabla - e\mathbf{A})\psi_2(\mathbf{x}) \tag{4.26}$$

$$\xrightarrow{\text{G.T.}} \int \mathrm{d}^3x\,\psi_1^*(\mathbf{x})e^{\frac{ie}{\hbar}\alpha}(-i\hbar\nabla - e\mathbf{A} + e\nabla\alpha)e^{-\frac{ie}{\hbar}\alpha}\psi_2(\mathbf{x}) \tag{4.27}$$

$$= \langle\psi_1|\,\hat{\mathbf{\Pi}}\,|\psi_2\rangle \tag{4.28}$$

Exercise 4.2 (Gauge covariant derivative)**.**
Show that, under a gauge transformation,

$$\hat{\mathbf{\Pi}} = -i\hbar\nabla - e\mathbf{A} \tag{4.29}$$

is a covariant derivative, i.e. $\hat{\mathbf{\Pi}}\psi$ *transforms as* ψ*.*

Exercise 4.3 (Gauge covariance of Schrödinger equation)**.**
Under a gauge transformation parametrized by α*, the Hamiltonian transforms as*

$$\hat{H} \xrightarrow{G.T.} H_\alpha = \frac{1}{2m}(\hat{\mathbf{p}} - e\mathbf{A} + e\nabla\alpha)^2 + e\Phi + e\partial_t\alpha. \tag{4.30}$$

Show that if ψ *solves the Schrödinger equation for* H *(*$\frac{i}{\hbar}\partial_t\psi = \hat{H}\psi$*) then* $\psi_\alpha \equiv e^{-\frac{ie}{\hbar}\alpha}\psi$ *solves the Schrödinger equation for* H_α*. In other words, prove the gauge covariance of the Schrödinger equation.*

The probability density $|\psi|^2$ is gauge invariant. In Quantum Mechanics, one can define a probability current $\mathbf{J}$ such that the following continuity equation holds:

$$\frac{\partial|\psi|^2}{\partial t} + \nabla\cdot\mathbf{J} = 0 \tag{4.31}$$

In regular quantum mechanics without an external EM field, we usually define the current

$$\tilde{\mathbf{J}} \equiv \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) = \frac{1}{2m}\left(\psi^*\hat{\mathbf{p}}\psi + \psi(\hat{\mathbf{p}}\psi)^*\right) \tag{4.32}$$

In the presence of an EM field, one can substitute $\hat{\mathbf{p}}$ with $\hat{\mathbf{\Pi}}$, the kinetic momentum, and see whether the continuity equation holds with

$$\mathbf{J} \equiv \frac{1}{2m}\left(\psi^*\hat{\mathbf{\Pi}}\psi + \psi(\hat{\mathbf{\Pi}}\psi)^*\right) = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) - \frac{e}{m}\mathbf{A}|\psi|^2 \tag{4.33}$$

Using the Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi = \left(\frac{1}{2m}\hat{\mathbf{\Pi}}^2 + e\Phi\right)\psi, \tag{4.34}$$

we have

$$i\hbar\frac{\partial|\psi|^2}{\partial t} = \psi^*\left(i\hbar\frac{\partial\psi}{\partial t}\right) - \psi\left(i\hbar\frac{\partial\psi}{\partial t}\right)^* \tag{4.35}$$

$$= \psi^*\left(\frac{1}{2m}\hat{\mathbf{\Pi}}^2 + e\Phi\right)\psi - \psi\left(\left(\frac{1}{2m}\hat{\mathbf{\Pi}}^2 + e\Phi\right)\psi\right)^* \tag{4.36}$$

$$= \frac{1}{2m}\left[\psi^*\hat{\mathbf{\Pi}}^2\psi - \psi\left(\hat{\mathbf{\Pi}}^2\psi\right)^*\right] \tag{4.37}$$

$$= -\frac{\hbar^2}{2m}\left[\psi^*\left(\nabla - \frac{ie}{\hbar}\mathbf{A}\right)^2\psi - \psi\left(\left(\nabla - \frac{ie}{\hbar}\mathbf{A}\right)^2\psi\right)^*\right] \tag{4.38}$$

Note now that

$$\left(\nabla - \frac{ie}{\hbar}\mathbf{A}\right)^2\psi = \nabla^2\psi - \frac{e^2}{\hbar^2}\mathbf{A}^2\psi - \frac{ie}{\hbar}\mathbf{A}\cdot\nabla\psi - \frac{ie}{\hbar}\nabla\cdot(\mathbf{A}\psi), \tag{4.39}$$

Using the above results, it can be shown that

$$\frac{\partial|\psi|^2}{\partial t} = -\frac{\hbar}{2mi}\left[\psi^*\nabla^2\psi - \psi\nabla^2\psi^* - \frac{2ie}{\hbar}\mathbf{A}\cdot\nabla|\psi|^2 - \frac{2ie}{\hbar}|\psi|^2\nabla\cdot\mathbf{A}\right] \tag{4.40}$$

$$= -\frac{\hbar}{2mi}\nabla\cdot[\psi^*\nabla\psi - \psi\nabla\psi^*] - \frac{e}{m}\nabla\cdot(\mathbf{A}|\psi|^2) \tag{4.41}$$

This is exactly $-\nabla\cdot J$! The continuity equation is therefore verified if we replace $\hat{\mathbf{p}}$ in the usual density current with the gauge-invariant kinetic momentum $\hat{\mathbf{\Pi}}$.

Charged particle in a constant magnetic field

Consider a constant magnetic field in the $\mathbf{e}_3$ direction: $\mathbf{B} = (0, 0, B)$. Recall that $\mathbf{B}$ is the curl of the vector potential $\mathbf{A}$. There are many solutions for $\mathbf{A}$ that satisfy this equation, which corresponds to the freedom to choose the gauge. A possible choice for $\mathbf{A}$ is

$$\mathbf{A} = \left(-\frac{By}{2}, \frac{Bx}{2}, 0\right) \tag{4.42}$$

Since we only want a constant $\mathbf{B}$ field, we can set $\Phi = 0$ from now on.

Given this potential, we have the following Hamiltonian:

$$H = \frac{1}{2m}\left[\left(\hat{p}_1 + \frac{eB}{2}\hat{y}\right)^2 + \left(\hat{p}_2 - \frac{eB}{2}\hat{x}\right)^2 + \hat{p}_3^2\right] \tag{4.43}$$

Clearly, translations along the x and y directions are a symmetry of the system since the $\mathbf{B}$ field is in the z direction. Moreover, translations are usually realized at the quantum level by considering $\hat{p}$ to be the generator of translations, i.e. $e^{\frac{i}{\hbar}a\hat{p}}\psi(x) = \psi(x + a)$. Without the magnetic field, we call "momentum" both the generator of translation and

the conjugate variable to the position (from $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$). In the rest of this section, we call "momenta" $\hat{p}_i$ the conjugate variable to the position, and we will see that the generators of translation will be different.

Indeed, note that in this case the momenta $\hat{p}_x$ and $\hat{p}_y$ do **not** commute with the Hamiltonian, since $\hat{H}$ depends on $\hat{x}$ and $\hat{y}$[1]. Therefore, the momenta $\hat{p}$ do not generate any symmetry, and we need to find other translation generators $\hat{T}_i$. These generators will need to commute with the Hamiltonian in order to correspond to the physical translation symmetry.

A sufficient condition to impose is

$$[\hat{T}_i, \hat{\Pi}_j] = 0, \tag{4.44}$$

since the Hamiltonian is built out of the kinetic momenta $\hat{\mathbf{\Pi}}$. A more intuitive reasoning for the above equation is that in the classical, nonrelativistic limit, $\mathbf{\Pi} = m\dot{\mathbf{x}}$. A translation should not change the velocity of the particle, hence the vanishing commutator above.

If we set the magnetic field to 0, we know that $\hat{T}_i = \hat{p}_i$, so we can define the Ansatz

$$\hat{\mathbf{T}} \equiv \hat{\mathbf{\Pi}} + \mathbf{F}(\hat{\mathbf{x}}). \tag{4.45}$$

The constraint (4.44) leads to

$$\begin{aligned} 0 &= [\hat{p}_i - eA_i + F_i, \hat{p}_j - eA_j] && (4.46)\\ &= ie\hbar(\underbrace{\partial_i A_j - \partial_j A_i}_{=\epsilon_{ijk}B_k}) + i\hbar\partial_j F_i && (4.47)\\ \implies F_i &= -e\epsilon_{ijk}x_j B_k + c_i. && (4.48) \end{aligned}$$

Note that the constants c_i are irrelevant. Indeed, they correspond to multiplying the state by a phase when translating it, which does not have a physical impact:

$$e^{i\alpha\cdot(\hat{\mathbf{T}}+\mathbf{c})}\,|\psi\rangle = \underbrace{e^{i\alpha\cdot\mathbf{c}}}_{\text{phase}} e^{i\alpha\cdot\hat{\mathbf{T}}}\,|\psi\rangle \tag{4.49}$$

Therefore, we have found the generators of translations!

$$\boxed{\hat{\mathbf{T}} = \hat{\mathbf{p}} - e(\mathbf{A} + (\mathbf{x}\wedge\mathbf{B}))} \tag{4.50}$$

A very important consequence is that translations do not commute:

$$[\hat{T}_i, \hat{T}_j] = \underbrace{[\hat{T}_i, \hat{\Pi}_j]}_{=0} + [\hat{T}_i, F_j] = -i\hbar\partial_i F_j = -i\hbar e\epsilon_{ijk}B_k \tag{4.51}$$

[1]Note that even if we had chosen a different gauge for $\mathbf{A}$, it would still depend on $\hat{x}$ or $\hat{y}$.

In particular, for our example with $\mathbf{B} = (0, 0, B)$, the translations along x and y do not commute:

$$[\hat{T}_x, \hat{T}_y] = -i\hbar eB \tag{4.52}$$

One can think of $\hat{T}_x$ and $\hat{T}_y$ as conjugate variables, just like $\hat{x}$ and $\hat{p}$ in standard quantum mechanics. In particular, since their commutator is a fixed complex number, they have an uncertainty relation. Furthermore, we can also show that

$$[\hat{\Pi}_x, \hat{\Pi}_y] = +i\hbar eB, \tag{4.53}$$

which means that the kinetic momenta along x and y can also be interpreted as a conjugate pair of variables.

What does the non-commutativity of translations mean? We have a symmetry group of translations which is obviously commutative, but the operators representing the group on the Hilbert space, the generators $\hat{T}_i$, are not commutative. In order to understand how this can occur, consider translating by a in the x direction, then by b in the y direction, then by $-a$ in the x direction, and finally by $-b$ in the y direction. In other words, our consecutive translations form a rectangle in the $x - y$ plane. This is realized at the quantum level as

$$\hat{U} \equiv e^{\frac{ib}{\hbar}\hat{T}_y} e^{\frac{ia}{\hbar}\hat{T}_x} e^{-\frac{ib}{\hbar}\hat{T}_y} e^{-\frac{ia}{\hbar}\hat{T}_x}. \tag{4.54}$$

Using the BCH formula (A.1), we can write

$$\hat{U} = \exp\left[-\frac{ib}{\hbar}\hat{T}_y - \frac{ia}{\hbar}\hat{T}_x + \frac{1}{2}\frac{ab}{\hbar^2}[\hat{T}_x, \hat{T}_y]\right] \exp\left[\frac{ib}{\hbar}\hat{T}_y + \frac{ia}{\hbar}\hat{T}_x + \frac{1}{2}\frac{ab}{\hbar^2}[\hat{T}_x, \hat{T}_y]\right] \tag{4.55}$$

$$= \exp\left[-\frac{i}{\hbar}eBab\right]. \tag{4.56}$$

This has a nice interpretation: $\Phi \Leftrightarrow Bab$ is the magnetic flux through the rectangle. Classically, $\hat{U}$ should be the identity, since we did 4 translations in a row to come back to the same place. However, in quantum mechanics, it is just a phase that only depends on the magnetic flux through the rectangle. Mathematically, we say that the group of translations is realized **projectively**. To summarize, if a quantum particle moves around a loop that borders a surface S, its phase changes by an angle equal to $-\frac{e}{\hbar}\Phi$, where Φ is the magnetic flux through S.

Classical motion:
The classical equation of motion is

$$m\ddot{\mathbf{x}} = e\dot{\mathbf{x}} \wedge \mathbf{B}, \tag{4.57}$$

and the solution can be written as

$$\begin{cases} x(t) = x_c + R\cos(\omega_c t) \\ y(t) = y_c - R\sin(\omega_c t) \end{cases}, \quad \omega_c = \frac{eB}{m}. \tag{4.58}$$

ω_c is called the cyclotron frequency. Now the translation generators T_x and T_y become

$$T_x = \Pi_x - eyB = m\dot{x} - m\omega_c y = -m\omega_c y_c \tag{4.59}$$

$$T_y = \Pi_y + exB = m\dot{y} + m\omega_c x = m\omega_c x_c. \tag{4.60}$$

Classically, (T_x, T_y) measure the position of the center of the circular orbits.

In the next lecture, we will look at two main consequences of the effects we discussed here: Landau Levels and the Aharonov-Bohm effect.

Summary of Lecture 11

- Charged particle in background EM field:

$$S = -mc^2 \int_\gamma \mathrm{d}\tau - \frac{e}{c}\int_\gamma A_\mu \mathrm{d}x^\mu = -\int \mathrm{d}t \left[mc^2\sqrt{1-\frac{\dot{x}^2}{c^2}} + e\Phi - e\mathbf{A}\cdot\dot{\mathbf{x}} \right]$$

- Gauge transformation:

$$\begin{aligned} A_\mu &\to A_\mu + c\partial_\mu \alpha \\ S &\to S - e\left[\alpha(x_f,t_f) - \alpha(x_i,t_i)\right] \\ \psi(x,t) &\to e^{-\frac{ie}{\hbar}\alpha(x,t)}\psi(x,t) \end{aligned}$$

- Hamiltonian and non-relativistic limit:

$$\begin{aligned} H &= \sqrt{(\mathbf{p}-e\mathbf{A})^2c^2 + m^2c^4} + e\Phi \\ H_{\text{non-rel}} &= \frac{1}{2m}(\underbrace{\mathbf{p}-e\mathbf{A}}_{=\boldsymbol{\Pi}})^2 + e\Phi, \end{aligned}$$

  where $\boldsymbol{\Pi}$ is the **kinetic momentum**.

- Charged particle in constant magnetic field $\mathbf{B} = (0,0,B)$. Generators of translations:

$$\hat{\mathbf{T}} = \hat{\mathbf{p}} - e(\mathbf{A} + (\mathbf{x}\wedge\mathbf{B}))$$

  Classically, T_x and T_y can be interpreted as the center of the circular orbits of the particle.

- Generators of translations and kinetic momentum do not commute among themselves:

$$\begin{aligned} [\hat{T}_x, \hat{T}_y] &= -i\hbar eB \\ [\hat{\Pi}_x, \hat{\Pi}_y] &= +i\hbar eB \end{aligned}$$

  Intuitively, translating a state around a closed path multiplies it by a phase $e^{-\frac{ie}{\hbar}\Phi}$, where Φ is the flux of the magnetic field passing through the closed path.

Lecture 12 - Landau Levels and Aharonov-Bohm effect

Landau Levels

We would now like to study the energy levels of a charged particle in a constant magnetic field. We will show that the energy levels are discrete, although they have a high degeneracy.

For simplicity, we choose the potential to be

$$\mathbf{A} = (-By, 0, 0), \quad \Phi = 0 \implies \mathbf{B} = (0, 0, B) \tag{4.61}$$

Using the definition of the non-relativistic hamiltonian (4.22), we can write

$$\hat{H} = \frac{1}{2m}\left((\hat{p}_1 + eB\hat{y})^2 + \hat{p}_2^2 + \hat{p}_3^2\right) \tag{4.62}$$

Translation invariance is manifest along x and z, but not along y since $\hat{H}$ depends explicitly on $\hat{y}$. In order to compute the spectrum of this Hamiltonian, we can construct explicit energy eigenfunctions $\psi(x, y, z)$. We define the Ansatz

$$\psi(x, y, z) = e^{\frac{i}{\hbar}(p_1 x + p_3 z)} F(y) \tag{4.63}$$

$$\implies \hat{H}\psi = \left[\frac{1}{2}m\Big(\underbrace{\frac{eB}{m}}_{\omega_c}\Big)^2\left(\hat{y} + \frac{p_1}{eB}\right)^2 + \frac{\hat{p}_2^2}{2m} + \frac{p_3^2}{2m}\right]\psi \tag{4.64}$$

Reorganizing the above and enforcing ψ to be an eigenfunction of $\hat{H}$ with energy E, we find

$$\underbrace{\left[\frac{\hat{p}_2^2}{2m} + \frac{1}{2}m\omega_c^2\left(\hat{y} + \frac{p_1}{eB}\right)^2\right]}_{\hat{H}_{\text{HO}}}\psi + \frac{p_3^2}{2m}\psi = E\psi \tag{4.65}$$

Note that the left-hand side corresponds to a (shifted[2]) harmonic oscillator in the y-direction! Therefore, the energy levels are

$$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right) + \frac{p_3^2}{2m} \tag{4.66}$$

Furthermore, the functions $F(y)$ are simply the energy wavefunctions of the harmonic oscillator, but centered at $y_c = -\frac{p_1}{eB}$. Therefore, we can write

$$\psi(x, y, z) = e^{\frac{i}{\hbar}(p_1 x + p_3 z)}\psi_n\left(y - y_c\right), \tag{4.67}$$

[2]Notice that the potential is centered around $y = -\frac{p_1}{eB}$.

where

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \tag{4.68}$$

and $H_n(x)$ are the Hermite polynomials. In order to visualize these states, we can compute $|\psi|^2$:

$$|\psi|^2 = |\psi_n(y - y_c)|^2, \tag{4.69}$$

which is just the probability density of the n-th level of the harmonic oscillator, but centered around y_c.

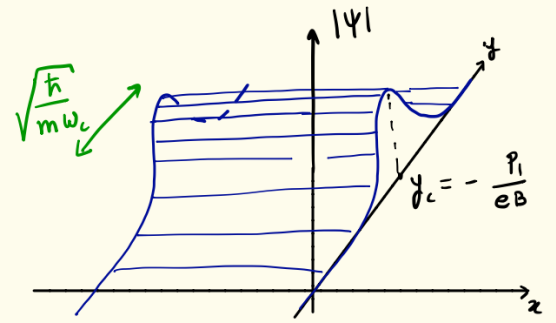


Figure 4.1: Probability density $|\psi|$ as a function of x, y for the case $n = 0$.

This seems to break the y-translation symmetry. However, if the Hamiltonian is degenerate (there are linearly independent states with the same energy), the y-translation symmetry only needs to hold in each subspace. We will discuss below that we can superpose states with different centers y_c but with the same energy to recover a y-translation symmetric state.

In order to study the degeneracy of the system, recall which quantum numbers we had to fix. We first set the momenta in the x and z direction, p_1 and p_3. Then, we had to use n to describe the energy level of the harmonic oscillator centered at y_c in the y-direction. We saw that y_c depends on the momentum in the x-direction as $y_c = -\frac{p_1}{eB}$. Therefore, if we fix (p_1, p_3, n) or alternatively (y_c, p_3, n), we have completely defined our wavefunction.

However, in the expression for the energy levels, p_1 (or alternatively y_c) does not appear. There is therefore a very large degeneracy corresponding to the fact that different states with the same p_3 and n, but centered at different y_c have the same energy. A general state in the n-th Landau level, with momentum p_3 along z is therefore given by

$$\psi(x, y, z) = e^{\frac{i}{\hbar}p_3 z} \int \mathrm{d}p_1 \, f(p_1) e^{\frac{i}{\hbar}p_1 x} \psi_n\left(y + \frac{p_1}{eB}\right) \tag{4.70}$$

Choosing $f(p)$ carefully, one can construct $\psi(x, y, z)$ to be an eigenstate of translations along x, y, but **not both**, since $[\hat{T}_1, \hat{T}_2] \neq 0$! Note that it is also possible to construct eigenstates of rotations around the z-axis.

Lastly, we can ask how many states are in a Landau level. Obviously, if we consider an infinite $x-y$ plane, there is infinitely many states in a level, one for each p_1 as argued above. However, if we consider the rectangle of side L_x and L_y, the momentum becomes quantized:

$$p_1 = \frac{2\pi\hbar}{L_x} m, \quad m \in \mathbb{Z} \quad \text{(periodic B.C.)} \tag{4.71}$$

Therefore,

$$y_c = -\underbrace{\frac{2\pi\hbar}{eBL_x}}_{\equiv \Delta y_c} m. \tag{4.72}$$

The centers are discrete! This is independent of the fact that L_y is fixed. If we had considered an infinite strip with $L_y \to \infty$, the centers would still be discretized in this way.

The number of states in the rectangle is then given by the length of the rectangle of the y-direction, divided by the space each state takes (assuming the rectangle to be much bigger than the spacing between states) :

$$N = \frac{L_y}{\Delta y_c} = \frac{eBL_xL_y}{2\pi\hbar} = \frac{\Phi}{2\Phi_0}, \tag{4.73}$$

where Φ is the magnetic flux, $\Phi = BL_xL_y$, and Φ_0 is the magnetic flux "quantum", $\frac{\pi\hbar}{e}$.

Aharonov-Bohm Effect

In classical electromagnetism, we learn that knowing the electric and magnetic fields in a region of interest gives a complete description of the physics in that region. However, using the formalism developed so far, we will show that this fails at the quantum level: some additional information about the system must be specified.

Consider a particle moving in $\mathbb{R}^3$, but with an infinite cylinder "removed" - the particle cannot go inside the cylinder. Mathematically, one could consider wavefunctions obeying the Schrödinger equation with boundary conditions $\psi(x, y, z) = 0$ at the boundary of the cylinder. Therefore, when computing the propagator, we must sum over paths which remain outside the cylinder:

$$K(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) = \int_{\substack{\text{outside} \\ \text{cylinder}}} \mathcal{D}[\mathbf{x}]\ e^{\frac{i}{\hbar}S[\mathbf{x}]} \tag{4.74}$$

Now imagine that we hide an infinite, continuous solenoid inside this cylinder. Classically, the magnetic field is uniform inside the solenoid, and vanishes outside. Therefore, since the particle is always outside the solenoid, it never "feels" any magnetic field, and we naively expect that the presence of a solenoid does not matter.

However, although the magnetic field vanishes outside the solenoid, the potential does not! Indeed, consider a surface S cutting through the solenoid, with boundary γ (see figure 4.2).

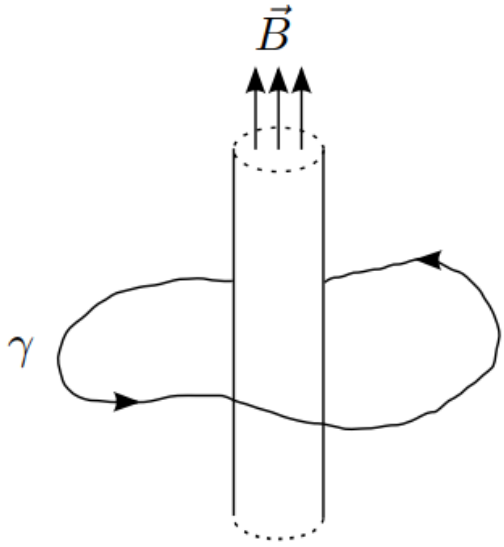


Figure 4.2: Infinite cylinder with constant uniform magnetic field inside. The path γ goes around the cylinder, and encloses a surface S through which there is a non-zero magnetic flux.

We can compute the circulation of the vector potential around γ in terms of the magnetic flux Φ inside the solenoid:

$$\int_{\gamma=\partial S} \mathbf{A} \cdot \mathrm{d}\mathbf{x} = \int_S \mathbf{B} \cdot \mathrm{d}S = \Phi. \tag{4.75}$$

Therefore, even though $\mathbf{B} = 0$ outside the cylinder, $\mathbf{A} \neq 0$! Classically, this does not have any effect since the system is entirely described by the $\mathbf{E}$ and $\mathbf{B}$ field, which are 0 outside the cylinder. Let us then investigate what happens at the quantum level.

Recall that the non-relativistic action for a charged particle in an EM field is given by

$$S = \int \mathrm{d}t \Big[\frac{1}{2} m \dot{\mathbf{x}}^2 - e\Phi + e\dot{\mathbf{x}} \cdot \mathbf{A} \Big] \tag{4.76}$$

In our case, $\Phi = 0$ and we can write

$$S = S_0 + e \int \mathbf{A} \cdot \mathrm{d}\mathbf{x}, \tag{4.77}$$

where S_0 is the free action. Therefore, if the charged particle is moving on a path γ, we have

$$e^{\frac{i}{\hbar} S[\gamma]} = e^{\frac{i}{\hbar} S_0[\gamma] + \frac{ie}{\hbar} \int_\gamma \mathbf{A} \cdot \mathrm{d}\mathbf{x}} \tag{4.78}$$

In the path integral, we sum these phases over different paths γ. Consider then the paths drawn in figure 4.3

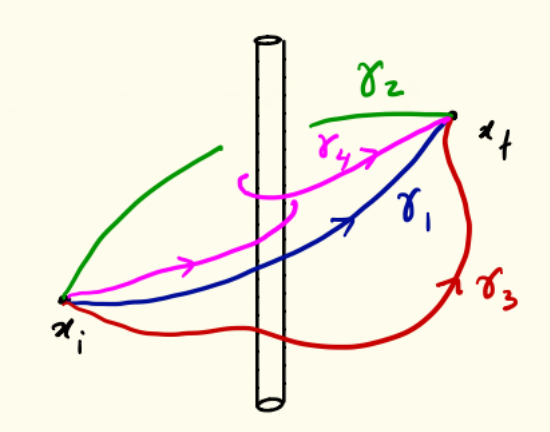


Figure 4.3: Different paths going from x_i to x_f that cannot be continuously deformed into each other due to the cylinder.

As a first example, we can compute the phase difference between the contribution from γ_1 and the contribution from γ_2:

$$\Delta\Phi_{12} = \frac{e}{\hbar}\left[\int_{\gamma_1} \mathbf{A}\cdot d\mathbf{x} - \int_{\gamma_2} \mathbf{A}\cdot d\mathbf{x}\right], \tag{4.79}$$

where $S_0[\gamma_1]$ and $S_0[\gamma_2]$ cancel out by symmetry (we choose γ_1 and γ_2 to be reflections of each other). Now the integral can be viewed as the circulation of $\mathbf{A}$ over the closed contour going from x_i to x_f following γ_1 and then back to x_i following γ_2. This circulation, as before, is the flux Φ!

$$\Delta\Phi_{12} = \frac{e\Phi}{\hbar} \tag{4.80}$$

Fundamentally, this arises because γ_1 and γ_2 are **topologically inequivalent** paths: they cannot be continuously deformed into each other due to the cylinder. Let us now look at topologically equivalent paths, γ_1 and γ_3. The phase difference $\Delta\Phi_{13}$ is now 0, since there is no magnetic flux through the surface enclosed by the path $\gamma_1 - \gamma_3$. Finally, we can study more complicated paths such as γ_4, and compute the phase difference $\Delta\Phi_{42}$. The closed path $\gamma_4 - \gamma_2$ goes around the solenoid twice, and therefore

$$\Delta\Phi_{42} = \frac{2e\Phi}{\hbar} \tag{4.81}$$

With these examples, we have understood that topologically inequivalent paths contribute different factors to the path integral.

To make this statement more precise, we associate a **winding number** n to each path. We will always compare paths to a basic "base" path, which we call γ_0 (this would

be γ_1 in figure 4.3). Then, if γ_n is a path with winding number n, we define

$$\oint_{\gamma_n - \gamma_0} \mathbf{A} \cdot \mathrm{d}\mathbf{x} \equiv n\Phi \tag{4.82}$$

Note that it is important to keep track of the orientation of the closed path to distinguish between positive and negative winding numbers.

Exercise 4.4 (Winding numbers)**.**
Convince yourself that in the example drawn in figure 4.3, γ_2 has winding number $n = -1$, γ_3 has $n = 0$ and γ_4 has $n = +1$.

Using this formalism, we can write

$$\frac{i}{\hbar} S[\gamma_n] = \frac{i}{\hbar} S_0[\gamma_n] + \frac{ie}{\hbar} \int_{\gamma_n} \mathbf{A} \cdot \mathrm{d}\mathbf{x} \tag{4.83}$$

$$= \frac{i}{\hbar} S_0[\gamma_n] + \frac{ie}{\hbar} n\Phi + i \underbrace{\frac{e}{\hbar} \int_{\gamma_0} \mathbf{A} \cdot \mathrm{d}\mathbf{x}}_{\equiv C}, \tag{4.84}$$

where C is just a constant real number depending on which γ_0 we choose.

The propagator can now be written as

$$K(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) = \sum_n \int_{\gamma_n} \mathcal{D}[x]\, e^{\frac{i}{\hbar} S_0[x] + in\frac{e\Phi}{\hbar}}, \tag{4.85}$$

where we discarded the overall phase corresponding to the base path (e^{iC}) as it does not have any observable effect on the wavefunction. Here, $\int_{\gamma_n}$ denotes the path integral over trajectories with fixed winding number n.

Note that this effect is periodic in Φ: if we increase Φ by $\frac{2\pi\hbar}{e}$, the physics is unaffected. In order to maximize this effect, we should therefore set $\Phi = \frac{\pi\hbar}{e} \equiv \Phi_0$. This factor is exactly the same as the one that appeared when counting the number of states in a Landau level.

The modified double-slit experiment:
Let us now study one system where this effect becomes physically evident: our favorite example, the double-slit experiment. Consider placing the solenoid between the two slits, so that there is a magnetic flux as indicated in figure 4.4

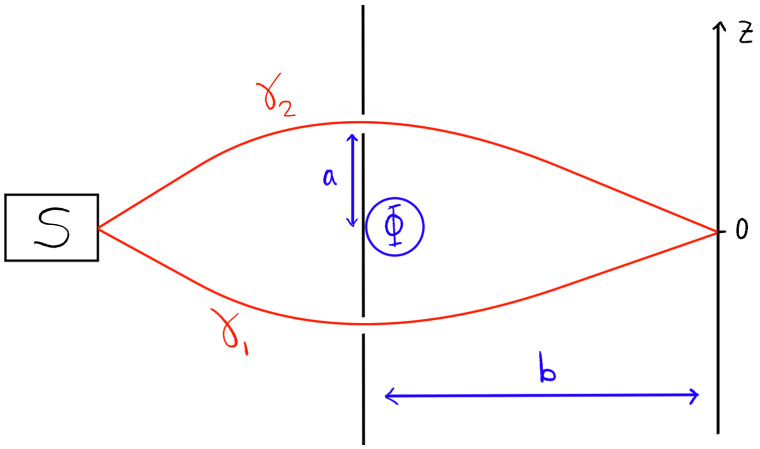


Figure 4.4: The experimental setup to test the Aharonov-Bohm effect. The double-slit experiment is modified to include a magnetic flux between the two slits, leading to topologically inequivalent trajectories γ_1 and γ_2.

Using equation (4.85), we can write

$$K(x_f, t_f; x_i, t_i) = K_1(x_f, t_f; x_i, t_i) + K_2(x_f, t_f; x_i, t_i)e^{-i\frac{e\Phi}{\hbar}} + \text{higher windings} \tag{4.86}$$

where K_i is the free propagator associated to the path γ_i. The higher windings contribute a negligible amount since they correspond to trajectories where the electron goes through the slits multiple times[3]. Then,

$$|K|^2 = |K_1|^2 + |K_2|^2 + 2\,\mathrm{Re}\left(K_1^* K_2 e^{-i\frac{e\Phi}{\hbar}}\right) \tag{4.87}$$

In the limit where $b \gg a \gg z$, we are really looking at the center of the interference pattern and we can neglect the decay of the amplitudes on the edges of the pattern. In this regime, we can assume free propagation and write

$$K_1 = Ae^{iqz}, \quad K_2 = Ae^{-iqz}, \tag{4.88}$$

where q is the momentum of the plane waves along z and the sign difference in the exponential comes from the fact that γ_1 comes from $-a$ and has positive momentum along z, while γ_2 comes from a and has negative momentum along z. In this approximation, we find

$$|K|^2 = 2|A|^2\left(1 + \cos\left(2qz + \frac{e\Phi}{\hbar}\right)\right). \tag{4.89}$$

Therefore, we expect the interference fringes **shift** with Φ! The effect is periodic under $\Phi \to \Phi + 2\Phi_0 n$, $n \in \mathbb{Z}$.

Through the Aharonov-Bohm effect, we have seen that $F_{\mu\nu}$ is not sufficient to describe electromagnetism. Indeed, different physical situations in a region can have the same

[3]We also neglected these trajectories in the original double slit experiment without the solenoid.

$F_{\mu\nu}$ in that region. We need to specify some other object as well to completely describe the physics, and that object must be gauge-invariant. As we have shown,

$$\oint \mathbf{A} \cdot \mathrm{d}\mathbf{x} \tag{4.90}$$

is gauge invariant, but it **overdescribes** electromagnetism! The right choice is the phase factor that appears in the path integral:

$$\exp\left(i\frac{e}{\hbar}\oint \mathbf{A} \cdot \mathrm{d}\mathbf{x}\right) \tag{4.91}$$

Together with $F_{\mu\nu}$, the above phase factor gives a complete description of electromagnetism! This formalism is used in lattice gauge theory, where there are phases $e^{i\varphi}$ on every link of the lattice.

Landau levels on a torus

Let us go back to the problem of a constant magnetic field orthogonal to the plane and consider periodic boundary conditions $x \sim x + L_x$ and $y \sim y + L_y$.

Classically, the system is translational invariant along x and along y, just like on an infinite plane. We can say that the symmetry group is $U(1) \times U(1)$. However, quantum mechanically, translations are broken to the discrete group $Z_N \times Z_N$ where N is the number of flux quanta through the torus. To see this consider the physical quantities:

$$W_x = \exp\left(i\frac{e}{\hbar}\int_0^{L_y} A_y(x,y)dy\right) \tag{4.92}$$

$$W_y = \exp\left(i\frac{e}{\hbar}\int_0^{L_x} A_x(x,y)dx\right) \tag{4.93}$$

Using Stokes theorem, it is easy to see that

$$W_{x+a} = W_x \exp\left(2\pi i N\frac{a}{L_x}\right), \qquad W_{y+b} = W_y \exp\left(2\pi i N\frac{b}{L_y}\right). \tag{4.94}$$

Therefore, we should not expect continuous translation invariance but only discrete $x \sim x + L_x/N$ and $y \sim y + L_y/N$.

It is possible to compute the wavefunctions for this problem (see arXiv:quant-ph/0007055). There are N orthogonal states in each Landau level. One can check that the gauge invariant density $\rho(x,y) = \sum_{i=1}^{N} |\psi_i(x,y)|^2$ of a Landau level depends on x, y in a way compatible with the discrete translational symmetry $Z_N \times Z_N$. [4]

Note that this quantum symmetry breaking effect is absent on a sphere. The Landau levels on a sphere preserve the full $SO(3)$ symmetry of the classical problem.

[4] As $N \to \infty$, the density $\rho(x,y)$ tends to the constant $N/(L_x L_y)$ exponentially fast.

Particle on a ring

As another example, consider a particle moving on a ring of radius R, with a solenoid at the center creating a magnetic flux Φ as showed in figure (4.5).

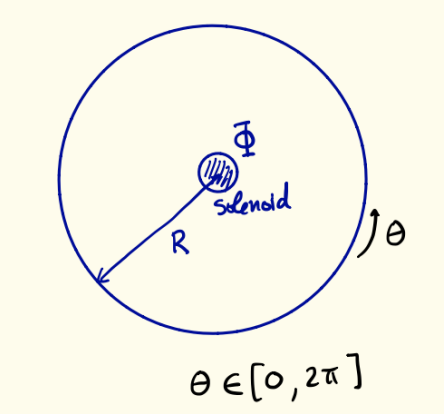


Figure 4.5: Particle moving around a solenoid with magnetic flux Φ.

Then,

$$\Phi = \int_\sigma \mathbf{B} \cdot \mathrm{d}\sigma = \int_{\partial\sigma} \mathbf{A} \cdot \mathrm{d}\mathbf{x} = 2\pi R A_\theta \tag{4.95}$$

where σ is a surface whose boundary $\partial\sigma$ is the ring. Now the Hamiltonian can be written as

$$H = \frac{1}{2m}\left[p_\theta - eA_\theta\right]^2 \tag{4.96}$$

$$= \frac{1}{2m}\left[-\frac{i\hbar}{R}\partial_\theta - \frac{e\Phi}{2\pi R}\right]^2, \tag{4.97}$$

where we used ∇ in polar coordinates. Now since θ is periodic, we **must** have

$$\psi_n(\theta) = e^{in\theta}, \quad n \in \mathbb{Z}, \tag{4.98}$$

which implies

$$E_n = \frac{\hbar^2}{2mR^2}\left[n - \frac{e\Phi}{2\pi\hbar}\right]^2 \tag{4.99}$$

$$= \frac{\hbar^2}{2mR^2}\left[n - \frac{\Phi}{2\Phi_0}\right]^2 \tag{4.100}$$

Therefore, the energy shift is periodic: the magnetic fluxes Φ and $\Phi + 2k\Phi_0$, for $k \in \mathbb{Z}$, give the same energy levels.

To summarize, the presence of the solenoid affects the energy levels of the particle in the ring, but this effect is periodic. The physics is therefore described by the phase

factor $e^{i\pi\frac{\Phi}{\Phi_0}}$!

Exercise 4.5 (Generalization of the particle on the ring)**.** *Consider again a particle on a ring, but with position-dependent EM potential* [5]*:*

$$H = \frac{1}{2m}\left[-i\hbar\partial_x - eA(x)\right]^2, \tag{4.101}$$

with fixed magnetic flux

$$\Phi = \int_0^L A(x)\,dx \tag{4.102}$$

Compute the energy eigenstates of the Hamiltonian (4.101). Hint: use the gauge transformation properties of the wavefunction ψ and A.

Magnetic Monopoles

This is based on an idea from Dirac [3]. Consider a semi-infinite thin solenoid as depicted in figure 4.6. At some point, the solenoid ends and the magnetic field "spreads out", as if it was created by a magnetic charge, which is called a **magnetic monopole**. Note that Maxwell's second law, $\nabla \cdot \mathbf{B} = 0$, is still satisfied as there is a non-zero magnetic flux coming from the solenoid.

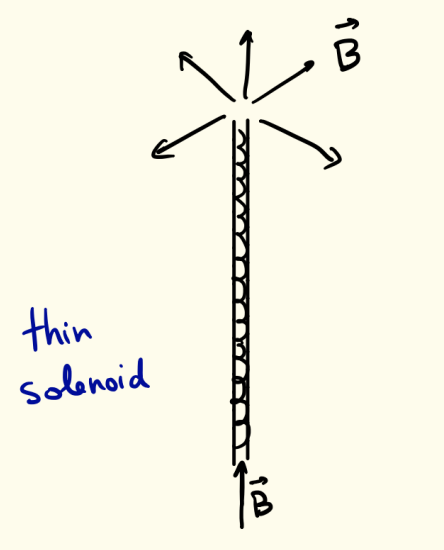


Figure 4.6: Semi-infinite thin solenoid acting as a magnetic monopole.

We call the semi-infinite thin solenoid a **Dirac string**, with magnetic field $\mathbf{B}_S$ inside the solenoid. The magnetic field of the monopole is denoted $\mathbf{B}_M$, and thus

$$\mathbf{B} = \mathbf{B}_S + \mathbf{B}_M \tag{4.103}$$

[5] This time, we consider the variable $x \in [0, L]$, with $L = 2\pi R$, but the system is the same as before if you identify $x = \theta R$. In this notation, periodicity implies $\psi(x) = \psi(x + L)$

Now we can use the Aharonov-Bohm effect to investigate whether the string is observable. **If the charge of every particle verifies**

$$\frac{e\Phi}{\hbar} = 2\pi n, \tag{4.104}$$

then the string is unobservable! Indeed, one can only "see" the string by using the Aharonov-Bohm effect and seeing interference pattern, since $\mathbf{B}_S$ vanishes everywhere outside the string. In other words, if the charges are quantized as in equation (4.104), then only the magnetic monopole field is observable. $\mathbf{B}_M$ behaves exactly like the electric field coming from a single charge:

$$\mathbf{B}_M = \frac{g_M}{4\pi r^2}\mathbf{e}_R, \tag{4.105}$$

where $g_M = \Phi$ is the magnetic charge.

Now the fact that $\nabla \cdot \mathbf{B} = 0$ is a kinematic fact: it only comes from $\mathbf{B} = \nabla \wedge \mathbf{A}$. Therefore, if a **single** monopole is observed, then all electric charges must be quantized:

$$e = \frac{2\pi\hbar}{g_M} n \tag{4.106}$$

This quantization condition can also be obtained in another way, which is the topic of exercise 34.

In nature, we observe every particle's charge to be integer multiple of the electron charge [6]. This is surprising, as there is no "group-theoretic" explanation for this quantization. For example, the quantization of the angular momentum directly comes from the structure of the associated $SU(2)$ algebra. In electromagnetism, the symmetry group is abelian and it does not impose any quantization.

Weak vs. Strong Coupling:
The strength of the electromagnetic interaction is set by the fine-structure constant:

$$\alpha = \frac{e^2}{4\pi\hbar c} \approx \frac{1}{137} \ll 1 \tag{4.107}$$

The EM interactions are therefore "weak". This means atoms are

- **Weakly bound:** $E_{\text{binding}} \sim \alpha^2 m_e \ll m_e$.
- **Large:** $r_B \sim \frac{1}{\alpha m_e} \gg \frac{1}{m_e}$.
- **Non-relativistic:** $v_e \sim \alpha c \ll c$.

[6] More precisely, every charge is an integer multiple of the down quark charge, which is equal to $\frac{1}{3}$ of the electron charge.

By charge quantization, the minimum possible g_M is

$$g_{\min} \equiv \frac{2\pi\hbar}{e}, \tag{4.108}$$

and therefore the analog of the fine-structure constant for magnetic monopoles would be very large:

$$\alpha_M \equiv \frac{g_M^2 c}{4\pi\hbar} \geq \frac{g_{\min}^2 c}{4\pi\hbar} = \frac{\pi\hbar c}{e^2} = \frac{1}{4\alpha} \approx 34 \gg 1 \tag{4.109}$$

Therefore magnetic monopoles must be strongly coupled!

Summary of Lecture 12

- Landau levels: constant $\mathbf{B} = (0, 0, B)$ implies energy levels

$$E_n = \hbar\omega_c \left(n + \frac{1}{2}\right) + \frac{p_3^2}{2m}.$$

  High degeneracy: many states with the same energy but centered at different y_c. Eigenstates of translations along x or y (but not both!) can be constructed by careful superposition.

- Number of states in a Landau level (on a finite rectangle with sides L_x, L_y):

$$N = \frac{\Phi}{2\Phi_0}, \quad \Phi = BL_xL_y, \quad \Phi_0 = \frac{\pi\hbar}{e}.$$

- Aharonov-Bohm effect: topologically inequivalent paths give rise to interference patterns. In modified double-slit experiment,

$$|K|^2 = 2|A|^2 \left(1 + \cos\left(2qz + \frac{e\Phi}{\hbar}\right)\right)$$

  $\rightarrow$ fringes shift with Φ.

- Particle in a ring: solenoid at center affects energy levels, but effect is periodic $\rightarrow$ described by a phase factor

$$\exp\left(i\pi\frac{\Phi}{\Phi_0}\right)$$

- Magnetic monopoles: if a single monopole is observed, **all** electric charges must be quantized

$$e = \frac{2\pi\hbar}{g_M}n$$

  Minimum possible g_M leads to strong coupling constant α_M.

Chapter 5

Quantum Chaos

Lecture 13 - Quantum Chaos

Special thanks to Behrang Tafreshi for carefully typing this lecture.

Classical Chaos

In classical physics, it is basically the idea of the butterfly effect. A small initial change can have a very big effect. Mathematically one can formulate that as the following. Consider a classical trajectory in phase space.

$$Y(t) = (x_i(t), p_i(t)), \tag{5.1}$$

where the dimension of Y is twice the number of degrees of freedom. Given two trajectories that start nearby $Y_1(0)$ and $Y_2(0)$:

$$|Y_1(0) - Y_2(0)| = \epsilon = \text{small}. \tag{5.2}$$

We find that $|Y_1(0) - Y_2(0)| \sim e^{\lambda t}\epsilon$, where λ is called the *Lyapunov* exponent. This is the idea of classical chaos. Of course there is much more to say, but our aim is to explain quantum chaos so we stop here and move on to the quantum version.

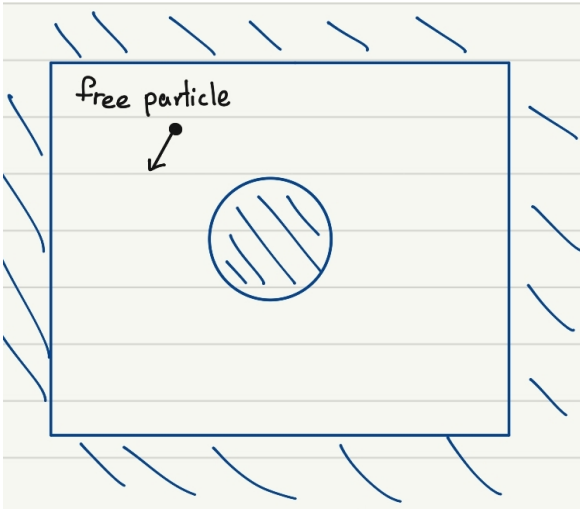
Quantum Chaos

A naive guess of what quantum chaos might be could be as follows. Let us start with two wave-functions which are very close and see how they evolve in time. Do they separate in time like the classical case? Of course not because time evolution is a unitary transformation in quantum mechanics. Therefore, the inner product between two states $\langle\psi_1|\psi_2\rangle$ is conserved.

However, there are many signatures of quantum chaos. One which we consider here is the statistical properties of the energy spectrum. Let us look at a very simple example which is also studied in classical chaos.

Example: (Sinai Billiards) A particle in a box can move with an impenetrable circle inside. This system is classically chaotic. But it is also chaotic quantum mechanically. You can watch animations of this online. Basically, if you concentrate on the eigenstates

of the system you will see a chaotic behaviour. But we will consider an even simpler signature of chaos which is the distribution of energy levels.



Basic idea: The quantum energy spectrum E_n in a small energy window around a large energy

$$E \gg \frac{\hbar^2}{mL^2}\,, \tag{5.3}$$

has the same statistical properties of the eigenvalues of a random matrix.

Notice that the spectral density is not universal. In fact, it is well described using semi-classical quantization. However, what will be universal is the way nearby energy levels are distributed. We will make this precise soon.

The history of the subject starts with Wigner and the distribution of the distance between consecutive energy levels of heavy nuclei. People started to see some universal behaviour and the conjecture shaped that for all chaotic quantum systems, in the high energy part of the spectrum, the statistics of the energy levels can be described using random matrices.

Random Matrix Theory

We are going to focus on the Gaussian Unitary Ensemble (GUE). Consider an ensemble of hermitian matrices with the following probability distribution :

$$P(M) \propto \exp\left(-\frac{1}{2}\mathrm{Tr}(M^2)\right) \prod_{i=1}^{N} dM_{ii} \prod_{i<j}^{N} d(\mathrm{Re}M_{ij}) d(\mathrm{Im}M_{ij}), \tag{5.4}$$

where M is a hermitian matrix. You can for example take real symmetric matrices which is a subset of the above. There are therefore different universality classes of quantum chaotic systems but there are a few of them. We want to find the distribution of the eigenvalues of this random matrix. It turns out that this distribution is not Gaussian.

Let us diagonalize the matrix :

$$M = U^\dagger diag(\lambda_1, \lambda_2, ..., \lambda_N)U. \tag{5.5}$$

The hard part would be to find the Jacobian of this change of variables:

$$\prod_{i=1}^{N} dM_{ii} \prod_{i<j}^{N} d(\mathrm{Re}M_{ij})d(\mathrm{Im}M_{ij}) = \mathcal{J} \prod_{i=1}^{N} d\lambda_i dU. \tag{5.6}$$

The result is that this Jacobian is as follows :

$$\mathcal{J} = \prod_{i<j}^{N} (\lambda_i - \lambda_j)^2. \tag{5.7}$$

Therefore :

$$P(\lambda_1, ..., \lambda_N) = c_N \exp\left(-\frac{1}{2}\sum_{i=1}^{N} \lambda_i^2\right) \prod_{i<j}^{N} (\lambda_i - \lambda_j)^2. \tag{5.8}$$

To compute the Jacobian we notice that the measure of the space of hermitian matrices M corresponds to the metric :

$$ds^2 = \mathrm{Tr}(dM^2). \tag{5.9}$$

This is basically a metric on $\mathbb{R}^{N^2}$. First note that this metric is invariant under conjugation by some fixed unitary matrix $M \to U_0 M U_0^\dagger$ with $U_0 \in U(N)$. Therefore, we can compute the determinant of the measure in the neighbourhood of the a diagonal matrix as any other matrix can be reached from this using one of the unitary matrices : $M = UDU^\dagger = e^{i\epsilon} D e^{-i\epsilon}$ where $\epsilon = \epsilon^\dagger$ and $D = \mathrm{diag}(\lambda_1, ..., \lambda_N)$. Since ϵ is very small, we can write :

$$M = D - i[\epsilon, D] + \mathcal{O}(\epsilon^2). \tag{5.10}$$

Therefore, we can see :

$$\begin{cases} M_{ii} = \lambda_i \\ M_{ij} = i\epsilon_{ij}(\lambda_i - \lambda_j) \quad i \neq j \end{cases} \tag{5.11}$$

We find that :

$$\prod_{i=1}^{N} dM_{ii} \prod_{i<j}^{N} d(\mathrm{Re}M_{ij})d(\mathrm{Im}M_{ij}) = \prod_{i=1}^{N} d\lambda_i \prod_{i<j}^{N} (\lambda_i - \lambda_j)^2 \prod_{i<j} d(\mathrm{Re}\epsilon_{ij})d(\mathrm{Im}\epsilon_{ij}). \tag{5.12}$$

But this last product is the term where we previously referred to as dU. But note that this is not exactly the space of unitary matrices. It is the space $U(N)/(U(1))^N$ because the diagonal elements do not contribute.

We want to take the $N \to \infty$ limit as the universality of quantum systems happens for this limit only! Note that we should calculate the normalization coefficient :

$$\int d\lambda_1 ... d\lambda_N P(\lambda_1, ..., \lambda_N) = 1 \tag{5.13}$$

This condition determines c_N which we will calculate in the process. For the time being however, we will continue by finding a nicer form for the Jacobian. The trick is to use the Vandermond determinant,

$$\begin{vmatrix} 1 & 1 & 1 & \dots & 1 \\ \lambda_1 & \lambda_2 & \lambda_3 & \dots & \lambda_N \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \lambda_1^{N-1} & \lambda_2^{N-1} & \lambda_3^{N-1} & \dots & \lambda_N^{N-1} \end{vmatrix} = \prod_{i<j}^{N} (\lambda_i - \lambda_j) \tag{5.14}$$

The proof of this equality can be done in 3 steps using basic properties of determinants.

1. Both sides are homogeneous polynomials of λ_is of degree $\frac{N(N-1)}{2}$. By homogeneous we mean that if you scale all the λ's by some parameter α, then the polynomial scales by $\alpha^{\frac{N(N-1)}{2}}$.

2. Both sides have the same zeros. If there exist i and j where $\lambda_i = \lambda_j$ then both sides are zero.

3. Both sides have the same overall coefficient. This can be checked by looking at one specific monomial.

Now consider having some definite monic polynomial $P_n(x) = x^n + \dots$ of degree n. Then we have that :

$$\begin{vmatrix} 1 & 1 & \dots & 1 \\ \lambda_1 & \lambda_2 & \dots & \lambda_N \\ \vdots & \vdots & \vdots & \vdots \\ \lambda_1^{N-1} & \lambda_2^{N-1} & \dots & \lambda_N^{N-1} \end{vmatrix} = \begin{vmatrix} 1 & 1 & \dots & 1 \\ \lambda_1 & \lambda_2 & \dots & \lambda_N \\ \vdots & \vdots & \vdots & \vdots \\ P_{N-1}(\lambda_1) & P_{N-1}(\lambda_2) & \dots & P_{N-1}(\lambda_N) \end{vmatrix} \tag{5.15}$$

This is possible because we can reduce the left hand side to the right hand side by subtracting the upper rows of the determinant which leave the total determinant invariant. We can do the same for the other rows as well and we end up with :

$$\begin{vmatrix} 1 & 1 & \dots & 1 \\ \lambda_1 & \lambda_2 & \dots & \lambda_N \\ \vdots & \vdots & \vdots & \vdots \\ \lambda_1^{N-1} & \lambda_2^{N-1} & \dots & \lambda_N^{N-1} \end{vmatrix} = \begin{vmatrix} P_0(\lambda_1) & P_0(\lambda_2) & \dots & P_0(\lambda_N) \\ P_1(\lambda_1) & P_1(\lambda_2) & \dots & P_1(\lambda_N) \\ \vdots & \vdots & \vdots & \vdots \\ P_{N-1}(\lambda_1) & P_{N-1}(\lambda_2) & \dots & P_{N-1}(\lambda_N) \end{vmatrix} \tag{5.16}$$

It is convenient to choose these polynomials to be the Hermite polynomials, $P_n(\lambda) = H_n(\lambda)$. Note that we are considering the monic Hermite polynomial. You can guess that the reason we chose Hermite polynomials is that we had Gaussian exponents and we love harmonic oscillators!

Therefore, we can write the distribution as :

$$\begin{aligned} P(\lambda_1, ..., \lambda_N) &= c_N \left[\det_{1 \le i,j \le N} \left[e^{-\frac{1}{4}\lambda_j^2} H_{i-1}(\lambda_j) \right] \right]^2 \\ &= \tilde{c}_N \left[\det_{1 \le i,j \le N} \left[\psi_{i-1}(\lambda_j) \right] \right]^2 = \tilde{c}_N (\det V)^2 \end{aligned} \tag{5.17}$$

where $\psi_n(x) = \frac{1}{(2\pi)^{1/4}\sqrt{n!}} e^{-(1/4)x^2} H_n(x)$ are the orthonormal wavefunctions of the harmonic oscillator and $V_{ij} = [\psi_{i-1}(\lambda_j)]$. Now we use the following :

$$P(\lambda_1, ..., \lambda_N) = \tilde{c}_N (\det V)^2 = \tilde{c}_N (\det V^T V). \tag{5.18}$$

However, we have :

$$(V^T V)_{ij} = \sum_{k=1}^{N} V_{ki} V_{kj} = \sum_{k=1}^{N} \psi_{k-1}(\lambda_i)\psi_{k-1}(\lambda_j) = K_N(\lambda_i, \lambda_j), \tag{5.19}$$

where we defined K_N through the above expression. Therefore, we have :

$$P(\lambda_1, ..., \lambda_N) = \tilde{c}_N \det_{i,j}[K_N(\lambda_i, \lambda_j)]. \tag{5.20}$$

Note that so far we have not really used the fact that we used Hermite polynomials. Now we are going to use that we chose the Hermite polynomials in particular. Now we use some identities to simplify this formula. Note that since we have the harmonic oscillator wavefunctions, we have :

$$\int dx \psi_n(x)\psi_m(x) = \delta_{nm}. \tag{5.21}$$

Now we can prove the following :

$$\int du K_N(x,u)K_N(u,y) = K_N(x,y). \tag{5.22}$$

Basically we just have to apply the orthonormality condition :

$$\begin{aligned} \int du K_N(x,u)K_N(u,y) &= \sum_{k=1}^{N}\sum_{l=1}^{N} \int \psi_{k-1}(x)\psi_{k-1}(u)\psi_{l-1}(u)\psi_{l-1}(y)du \\ &= \sum_{k=1}^{N}\sum_{l=1}^{N} \psi_{k-1}(x)\psi_{l-1}(y)\delta_{kl} \\ &= \sum_{k=1}^{N} \psi_{k-1}(x)\psi_{k-1}(y) = K_N(x,y). \end{aligned} \tag{5.23}$$

Furthermore, the following is easy to see :

$$\int K_N(x,x)dx = \sum_{k=1}^{N} \int dx (\psi_{k-1}(x))^2 = \sum_{k=1}^{N} 1 = N. \tag{5.24}$$

Now think of the big picture of what we have up until now. We have the distribution of all λ's which is a lot of information. So much so that it is hard to analyze! It would be good if we could integrate out some of them to reduce the distribution function to $P(\lambda_i)$ for example. The following identity helps us with this.

$$\int d\lambda_n \det_{1\le i,j\le n}[K_N(\lambda_i,\lambda_j)] = (N-n+1) \det_{1\le i,j\le n-1} K_N(\lambda_i,\lambda_j). \tag{5.25}$$

In order to prove this identity, we use the following notation. By $\det_{!i,!j} K_N(\lambda_i, \lambda_j)$ we mean the determinant of the submatrix with the ith and jth column omitted. Note that in all the cases we are only considering the $n \times n$ matrix only. Therefore, we have :

$$\begin{aligned}
&\det_{1\leq i,j\leq n} K_N(\lambda_i, \lambda_j) = \sum_{t=1}^{n} (-1)^{n+t} [\det_{!t,!n} K_N(\lambda_i, \lambda_j)] K_N(\lambda_t, \lambda_n) \\
&= (-1)^{2n} [\det_{!n,!n} K_N(\lambda_i, \lambda_j)] K_N(\lambda_n, \lambda_n) + \sum_{t=1}^{n-1} (-1)^{n+t} [\det_{!t,!n} K_N(\lambda_i, \lambda_j)] K_N(\lambda_t, \lambda_n) \\
&= [\det_{!n,!n} K_N(\lambda_i, \lambda_j)] K_N(\lambda_n, \lambda_n) \\
&+ \sum_{t=1}^{n-1} \sum_{l=1}^{n-1} (-1)^{2n+t+l-1} [\det_{\substack{(!t,!n)\\(!n,!l)}} K_N(\lambda_i, \lambda_j)] K_N(\lambda_t, \lambda_n) K_N(\lambda_n, \lambda_l)
\end{aligned} \tag{5.26}$$

Basically what we did was to first expand the determinant for the last column and then expand the sub-determinant for the last row. Now if we integrate over λ_n and use the 2 previous identities we get :

$$\begin{aligned}
&\int d\lambda_n \det_{1\leq i,j\leq n} [K_N(\lambda_i, \lambda_j)] \\
&= \int d\lambda_n [\det_{!n,!n} K_N(\lambda_i, \lambda_j)] K_N(\lambda_n, \lambda_n) \\
&+ \sum_{t=1}^{n-1} \sum_{l=1}^{n-1} (-1)^{t+l-1} [\det_{\substack{(!t,!n)\\(!n,!l)}} K_N(\lambda_i, \lambda_j)] K_N(\lambda_t, \lambda_n) K_N(\lambda_n, \lambda_l) \\
&= N [\det_{!n,!n} K_N(\lambda_i, \lambda_j)] - \sum_{t=1}^{n-1} \sum_{l=1}^{n-1} (-1)^{t+l} [\det_{\substack{(!t,!n)\\(!n,!l)}} K_N(\lambda_i, \lambda_j)] K_N(\lambda_t, \lambda_l) \\
&= N [\det_{!n,!n} K_N(\lambda_i, \lambda_j)] - \sum_{t=1}^{n-1} \det_{1\leq i,j\leq n-1} [K_N(\lambda_i, \lambda_j)] \\
&= (N - n + 1) \det_{1\leq i,j\leq n-1} [K_N(\lambda_i, \lambda_j)].
\end{aligned} \tag{5.27}$$

We can use this formula to find $\tilde{c}_N$. If we use it N times, we get :

$$\int d\lambda_1 ... d\lambda_N \det_{i,j} [K_N(\lambda_i, \lambda_j)] = N! \tag{5.28}$$

Therefore we have $\tilde{c}_N = \frac{1}{N!}$. Now if we use the formula to integrate over $N - 1$ of the eigenvalues, we get :

$$P(\lambda) = \int d\lambda_2 ... d\lambda_N P(\lambda_1, ..., \lambda_N) = \frac{1}{N} K_N(\lambda, \lambda) = \frac{1}{N} \sum_{k=0}^{N-1} |\psi_k(\lambda)|^2. \tag{5.29}$$

This is the sum of probability distributions of the first N levels of the harmonic oscillator. In the large N limit, we can use the semi-classical approximation. Think of this as a harmonic oscillator with the first N levels occupied. For the final level we have :

$$\frac{\partial^2}{\partial x^2}\psi_{N-1}(x) + \frac{1}{4}x^2\psi_{N-1}(x) = \left[\frac{1}{2} + (N-1)\right]\psi_{N-1}. \tag{5.30}$$

Semi-classically we have :

$$p^2 + \frac{1}{4}x^2 = N - \frac{1}{2}. \tag{5.31}$$

Therefore the probability distribution is (see Figure 5.1):

$$P(\lambda) \propto 2P_{max}(x = \lambda). \tag{5.32}$$

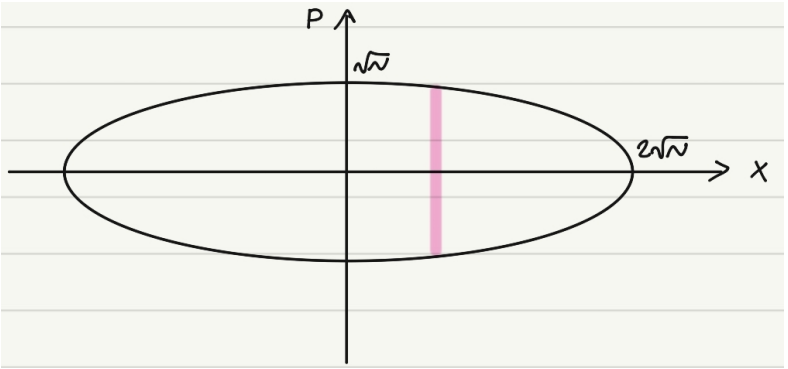


Figure 5.1: Phase space of the Harmonic Oscillator

$$\Rightarrow P(\lambda) = \begin{cases} \frac{\sqrt{N-\frac{1}{2}-\frac{\lambda^2}{4}}}{\pi N} & |\lambda| \leq 2\sqrt{N-\frac{1}{2}} \\ 0 & |\lambda| > 2\sqrt{N-\frac{1}{2}} \end{cases} \tag{5.33}$$

Since we are taking the large N limit, we can even omit the $\frac{1}{2}$ in the distribution. This is called Wigner's semi-circular law. This was fun but it is not a universal feature! Different systems have different density of states. However, we wanted to look at universal properties which is the statistics of nearby levels. In physicist terms, we want to know how nearby levels repel. This means that in order to look at nearby states, we need two pairs of eigenstates.

$$\begin{aligned} P(\lambda_1, \lambda_2) &= \int d\lambda_3 ... d\lambda_N P(\lambda_1, ..., \lambda_N) \\ &= \frac{1}{N(N-1)} \begin{vmatrix} K_N(\lambda_1, \lambda_1) & K_N(\lambda_1, \lambda_2) \\ K_N(\lambda_2, \lambda_1) & K_N(\lambda_2, \lambda_2) \end{vmatrix} \end{aligned} \tag{5.34}$$

Again we must use some identities. The first one is called the Christoffel-Darboux :

$$K_N(x, y) = \sum_{k=0}^{N-1} \psi_k(x)\psi_k(y) = \sqrt{N}\frac{\psi_N(x)\psi_{N-1}(y) - \psi_N(y)\psi_{N-1}(x)}{x - y}. \tag{5.35}$$

For the proof we use the following identity of harmonic oscillator wavefunctions :

$$x\psi_k(x) = \sqrt{k+1}\psi_{k+1}(x) + \sqrt{k}\psi_{k-1}(x). \tag{5.36}$$

The proof is the as follows :

$$\begin{aligned}(x-y)K_N(x,y) &= (x-y)\sum_{k=0}^{N-1}\psi_k(x)\psi_k(y) \\ &= \sum_{k=1}^{N-1}\left(\sqrt{k+1}\psi_{k+1}(x)\psi_k(y) + \sqrt{k}\psi_{k-1}(x)\psi_k(y)\right) \\ &- \sum_{k=1}^{N-1}\left(\sqrt{k+1}\psi_{k+1}(x)\psi_k(y) + \sqrt{k}\psi_{k-1}(x)\psi_k(y)\right).\end{aligned} \tag{5.37}$$

After cancelling the terms we get the wanted identity. The last non-trivial element of our discussion is what we exactly mean by the large N limit. Remember the semi-circular law. We have N eigenvalues inside the interval $[-\sqrt{N}, \sqrt{N}]$. Therefore the spacing of the eigenvalues is of order $\Delta\lambda \sim \frac{\sqrt{N}}{N} = \frac{1}{\sqrt{N}}$. As a result, the eigenvalues get densely packed when N goes to infinity. In particular if we choose some value of $x \in [-2, 2]$, what is the eigenvalue spacing of $x\sqrt{N}$? The answer is $\frac{1}{P\left(x\sqrt{N}\right)N}$. In mathematical terms, we take the following limit :

$$\begin{aligned}&N \to \infty \\ &\lambda_1 = \sqrt{N}x \\ &\lambda_2 - \lambda_1 = \frac{2\pi z}{\sqrt{4-x^2}\sqrt{N}}\end{aligned} \tag{5.38}$$

where z is fixed and this is chosen so that $z = 1$ corresponds to consecutive eigenvalues. This is very important as we want to see the correlation of the eigenvalues and therefore we need to be in the right scale to see it.

$$P(\lambda_1, \lambda_2) \to \frac{N}{N-1}P(\lambda_1)P(\lambda_2) - \frac{K_N(\lambda_1, \lambda_2)}{N(N-1)}, \tag{5.39}$$

where $P(\lambda) = \frac{1}{N}K_N(\lambda, \lambda)$. We now use the Christoffel-Darboux (eq. 5.35) formula for the second term and use the semiclassical approximation as we are taking the large N limit. The WKB approximation is :

$$\psi_N^{WKB}(x) = \frac{1}{\sqrt{\pi}\left(N - \frac{x^2}{4}\right)^{1/4}}\cos\left(\int_0^x \sqrt{N - \frac{y^2}{4}}dy - N\frac{\pi}{2}\right). \tag{5.40}$$

If you plug it into the Christoffel-Darboux formula, and take the large N limit, you get the following :

$$P(\lambda_1, \lambda_2) \to P(\lambda_1)^2\left[1 - \left(\frac{\sin(\pi z)}{\pi z}\right)^2\right]. \tag{5.41}$$

This function is the sine kernel. Let us state our final result in its full glory :

$$P(\lambda_1, \lambda_2) \to P(\lambda_1)^2 \left[1 - \left(\frac{\sin(\pi z)}{\pi z}\right)^2\right], \tag{5.42}$$

in the large N limit where $z = \lim_{N\to\infty}(\lambda_1 - \lambda_2)P(\lambda_1)N$.

The plot of this function you can see in Figure 5.2. You see that the peaks correspond

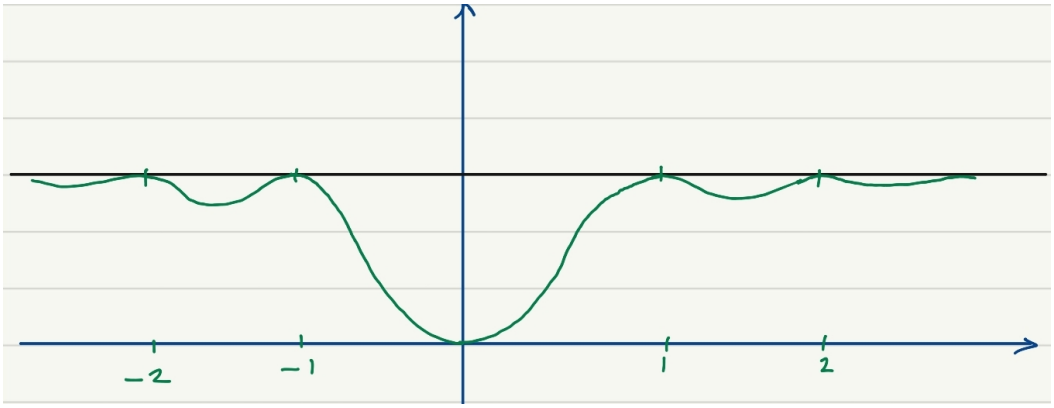


Figure 5.2: Sine Kernel Plot

to a crystal of eigenvalues which are all spaced by one! Of course it is not a rigid crystal as it is a random thing but you get the picture. The most important feature is the gap between -1 and 1 where it is very hard to find two eigenvalues very close to each other. This is called level repulsion! This is the universal feature. This is expected to be valid in any quantum chaotic system :

$$\boxed{\frac{\rho(E_1, E_2)}{\rho(E_1)\rho(E_2)} \xrightarrow[\rho(E_1)\to\infty]{(E_1-E_2)\rho(E_1)=z \quad \text{fixed}} 1 - \left(\frac{\sin(\pi z)}{\pi z}\right)^2} \tag{5.43}$$

We emphasize that this universal behaviour is true for Gaussian Unitary matrices, but there are only a few universality classes in general.

Appendix A

Mathematics

In this appendix, we summarize some of the mathematical tools used in the main text.

A.1 Baker-Campbell-Hausdorff and Zassenhaus formulas

For two non-commuting operators X and Y, we have the **BCH formula**:

$$e^X e^Y = e^Z, \tag{A.1}$$

where

$$Z = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[X,[X,Y]] - \frac{1}{12}[Y,[X,Y]] + \dots \tag{A.2}$$

The **Zassenhaus formula** gives the reverse direction:

$$e^{t(X+Y)} = e^{tX} e^{tY} e^{-\frac{t^2}{2}[X,Y]} e^{\frac{t^3}{6}(2[Y,[X,Y]]+[X,[X,Y]])}, \quad t \in \mathbb{C} \tag{A.3}$$

A.2 Complex analysis theorems

Cauchy's theorem
Let $U \in \mathbb{C}$ be a simply connected region $U \subset \mathbb{C}$ and $f(z)$ a holomorphic function on U. Then, for any closed curve $\gamma \subset U$, we have

$$\oint_\gamma dz\, f(z) = 0 \tag{A.4}$$

Residue theorem
Let $U \in \mathbb{C}$ be a simply connected region $U \subset \mathbb{C}$ and $f(z)$ a holomorphic function on $U \backslash \{z_1, z_2, \dots, z_n\}$. Then, for any closed curve $\gamma \subset U$ avoiding the singular points $z_1, z_2, \dots, z_n$, we have

$$\oint_\gamma dz\, f(z) = 2\pi i \sum_{k=1}^{n} \mathrm{Res}(f, z_k)\,. \tag{A.5}$$

If the singular point z_k is a pole of order q then the residue is given by

$$\mathrm{Res}(f, z_k) = \frac{1}{(q-1)!} \lim_{z \to z_k} \frac{d^{q-1}}{dz^{q-1}} (z - z_k)^q f(z) \tag{A.6}$$

A.3 Fourier transform

In our conventions, the Fourier transform of a function $f(\mathbf{x})$, where $\mathbf{x} \in \mathbb{R}^n$ is given by

$$\tilde{f}(\mathbf{k}) = \int_{\mathbb{R}^n} \mathrm{d}^n x \, f(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} \,, \tag{A.7}$$

where $\mathbf{k} \cdot \mathbf{x}$ is the Euclidean scalar product. The inverse transform is then

$$f(\mathbf{x}) = \int_{\mathbb{R}^n} \frac{\mathrm{d}^n k}{(2\pi)^n} \, \tilde{f}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} \,. \tag{A.8}$$

For functions of space and time (spacetime) we shall use the convention

$$\begin{aligned} \tilde{f}(\mathbf{k}, \omega) &= \int_{\mathbb{R}^4} \mathrm{d}^3 x \, \mathrm{d}t \, f(\mathbf{x}, t) e^{i\omega t - i\mathbf{k}\cdot\mathbf{x}} \\ f(\mathbf{x}, t) &= \int_{\mathbb{R}^4} \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{\mathrm{d}\omega}{2\pi} \, \tilde{f}(\mathbf{k}, \omega) e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} \end{aligned}$$

Appendix B

Computational details

B.1 No degenerate energy levels in 1D quantum mechanics

Given a time-independent potential $V(x)$, the wavefunctions verify the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \tag{B.1}$$

Assume there are 2 independent solutions with energy E, ψ_1 and ψ_2. We can compute the Wronskian

$$W = \psi_1\psi_2' - \psi_1'\psi_2 = \text{constant} \tag{B.2}$$

Assuming that the wavefunctions are normalized and well behaved, we can take the $x \to \infty$ limit of the above and both ψ_1 and ψ_2 will vanish. Therefore, $W = 0$ and we have

$$\frac{\psi_1'}{\psi_1} = \frac{\psi_2'}{\psi_2} \tag{B.3}$$

$$\implies \ln(\psi_1) = \ln(\psi_2) + c \tag{B.4}$$

$$\implies \psi_2 = \tilde{c}\psi_1, \tag{B.5}$$

which shows us that the two wavefunctions are proportional to one another. These do not differ physically, and we have thus proven that there are no degenerate states in 1D quantum mechanics (for a time-independent potential).

B.2 Derivatives acting on δ functions

In the study of Feynman diagrams, one often encounters integrals containing derivatives acting on delta functions. Although this can seem confusing at first, they are actually easy to deal with, as they can always be removed through integration by parts. For

example, we used this trick in equation (2.51):

$$\begin{aligned}
S_E &= \frac{1}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2\, x(\tau_1) O(\tau_1,\tau_2) x(\tau_2) \\
&= \frac{1}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2\, x(\tau_1) \left[-m\frac{\partial^2}{\partial\tau_1^2} + m\omega^2\right] \delta(\tau_1-\tau_2) x(\tau_2) \\
&= -\frac{m}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2\, x(\tau_1) \frac{\partial^2}{\partial\tau_1^2}\delta(\tau_1-\tau_2) x(\tau_2) + \frac{1}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, m\omega^2 x^2(\tau) \\
&= -\frac{m}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2\, \frac{\partial^2 x(\tau_1)}{\partial\tau_1^2}\delta(\tau_1-\tau_2) x(\tau_2) + \frac{1}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, m\omega^2 x^2(\tau) \\
&= \frac{1}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, x(\tau) \left[-m\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + m\omega^2\right] x(\tau)
\end{aligned}$$

B.3 Phases from analytic continuation

We show below that the number of negative eigenvalues n_- from the Gelfand-Yaglom formula is equal to the number of zeroes of $\psi_0(t)$, using complex analysis methods.

- Naively, we could have written

$$I[x_c] = \sqrt{\frac{m}{2\pi i\hbar\psi_0(t_f)}}, \tag{B.6}$$

  for t_f very close to t_i. Indeed, in that regime, $\psi_0(t_f) > 0$ because of the initial conditions $\psi_0(t_i) = 0$ and $\dot{\psi}_0(t_i) = 1$.

  You can think of t_f as being an external parameter that we can modify, and for each value of t_f we will get a value of $I[x_c]$. Since $I[x_c]$ can be complex, increasing t_f (starting from $t_f = t_i + \delta$, $\delta \ll 1$) will give us "trajectories" in the complex plane.

  Now for general t_f, we expect $\psi_0(t)$ to be an oscillatory function by analogy with the harmonic oscillator case (here the frequency is time-dependent but the oscillatory behavior remains). As we increase t_f, we therefore expect that for some value of t_f, $\psi_0(t_f) = 0$. If we keep increasing t_f, we expect $\psi_0(t_f)$ to be negative by continuity. This means that there will be a phase $e^{-i\frac{\pi}{2}}$ appearing in front, which is very reminiscent of equation (3.11).

- Let us be more precise. Given some t_f, we know that $\psi_0(t)$ is an oscillatory function in the range $[t_i, t_f]$. Let us label by t_k, $k = 1, \ldots$ its zeros. In formula (B.6), we see that this leads to the divergence of $I[x_c]$, which is problematic. More precisely,

$$I[x_c] \propto \frac{1}{\sqrt{\psi_0(t_f)}}, \tag{B.7}$$

which means that if we think of $I[x_c]$ as a function of t_f, it has a branch point at each t_k (the zeros of $\psi_0(t)$). However, we should be thinking of Minkowski "real" time as the Wick rotation of Euclidean time, with $\tau = it(1 - i\epsilon)$[1]. Therefore, we do not technically hit the branch points at $t_f = t_k$ (see figure B.1).

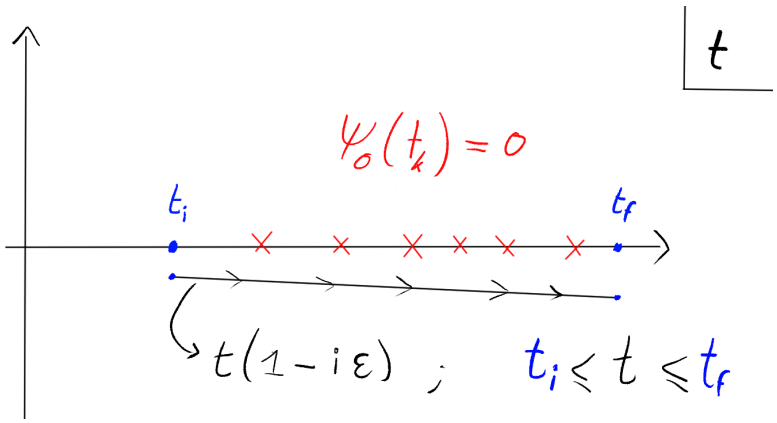


Figure B.1

- Given this, we can make our formulas more precise by sending

$$\psi_0(t_f) \to \psi_0(t_f(1 - i\epsilon)) \approx \psi_0(t_f) - i\epsilon\dot{\psi}_0(t_f) \tag{B.8}$$

Therefore, as we increase t_f, we do not hit the branch points of $I[x_c]$, but we rather go around it (see figure B.2). Indeed, for very small t_f, we have $\psi_0(t_f) \approx \psi_0(t_i) = 0$ and $\dot{\psi}_0(t_f) \approx \dot{\psi}_0(t_i) = 1$, so with the $i\epsilon$ prescription we have $\psi_0(t_f) \approx -i\epsilon$. Now as we increase t_f, the real part increases, and we reach the real line when the imaginary part is 0, i.e. at the first maximum of $\psi_0(t_f)$. Then, the real part decreases again until we reach $\psi_0(t_f) = 0$, which was causing problems before. However now there is a nonzero imaginary part due to the $-i\epsilon\dot{\psi}_0(t_f)$!

[1]For more details about the $i\epsilon$ prescription, recall the discussion at the end of Lecture 5.

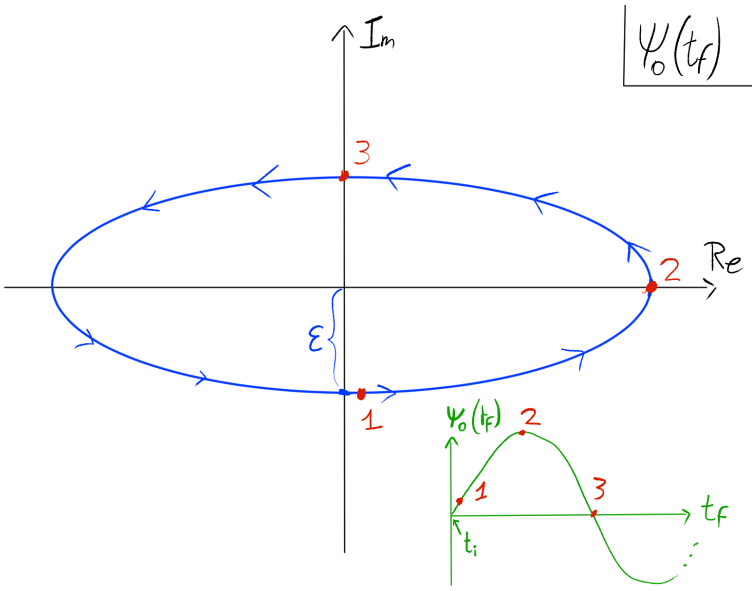


Figure B.2

- We can now finally understand the phase factor! We know that $I[x_c] \propto \frac{1}{\sqrt{\psi_0(t_f)}}$, so let us study what happens when we go around the branch point. The function $\sqrt{z}$ has a branch cut (we can choose it to be on the negative real axis for convenience, which means that complex numbers have argument $\theta \in]-\pi, \pi[$), which leads to a discontinuity. Indeed, let $x_\pm$ be complex numbers with negative real parts and small positive/negative imaginary parts:

$$x_\pm = -r \pm i\epsilon, \quad r > 0 \tag{B.9}$$

Then,

$$\frac{1}{\sqrt{x_+}} = (-r + i\epsilon)^{-1/2} = (|r|e^{i(\pi-\tilde{\epsilon})})^{-1/2} \approx \frac{e^{-i\frac{\pi}{2}}}{\sqrt{|r|}} \tag{B.10}$$

$$\frac{1}{\sqrt{x_-}} = (-r - i\epsilon)^{-1/2} = (|r|e^{i(-\pi+\tilde{\epsilon})})^{-1/2} \approx \frac{e^{i\frac{\pi}{2}}}{\sqrt{|r|}} \tag{B.11}$$

we therefore see that crossing the branch cut (from above) leads to a multiplication by a phase $e^{i\pi}$.

The number of times this happens can be related to the number of zeros of $\psi_0(t)$ in $[t_i, t_f]$ for a given t_f. Indeed, we cross the branch cut for each minimum of ψ_0, and the number of minima ($n_{\min}$) of ψ_0 is half the number of zeros (n_0) of ψ_0. Therefore, we find the phase factor

$$e^{i\pi n_{\min}} = e^{i\frac{\pi}{2}n_0} \tag{B.12}$$

Therefore, we have

$$\frac{1}{\sqrt{\psi_0(t_f)}} e^{i\frac{\pi}{2}n_0} = \frac{1}{\sqrt{|\psi_0(t_f)|}} \tag{B.13}$$

which gives us back the original formula we found using Gelfand-Yaglom:

$$I[x_c] = e^{-i\frac{\pi}{2}n_0} \sqrt{\frac{m}{2\pi i\hbar|\psi_0(t_f)|}} \tag{B.14}$$

where now the integer in the exponential is the number of zeroes of ψ_0 instead of the number of negative eigenvalues of the differential operator.

B.4 Multiple saddle points semiclassical spectral density computation

We want to compute the semiclassical approximation for the spectral density by using formula (3.95):

$$K_{sc}(E;x_f,x_i)=\sum_n \frac{e^{-i\frac{\pi}{2}N_n}}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\int_{x_i}^{x_f} \mathrm{d}x_{(n)}\, p(x)} \tag{B.15}$$

To clarify the notation, we consider the trajectories shown in figure (B.3). We will first compute the contribution from the green paths, which are initially going towards x_f, and then the contribution from pink paths:

$$K_{sc}(E;x_f,x_i)=K_{sc}^{\text{green}}(E;x_f,x_i)+K_{sc}^{\text{pink}}(E;x_f,x_i) \tag{B.16}$$

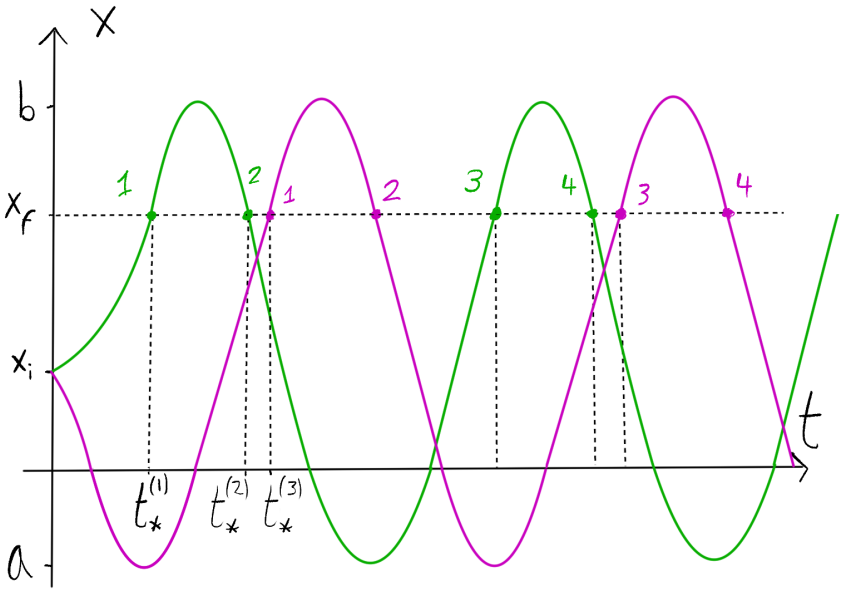


Figure B.3: Different oscillating paths corresponding to different saddle points. Green paths are labelled by integers independently from pink paths.

Since the paths are oscillating, we can deduce the contribution from the $(n+2)$'th path from the n'th path. Indeed, we have the following recursive identity:

$$\int_{x_i}^{x_f} p(x)\,\mathrm{d}x_{(n+2)}=\int_{x_i}^{x_f} p(x)\,\mathrm{d}x_{(n)}+\underbrace{2\int_a^b p(x)\,\mathrm{d}x}_{=\Omega(E)} \tag{B.17}$$

Furthermore, we can relate the second path to the first as

$$\int_{x_i}^{x_f} p(x)\,\mathrm{d}x_{(2)}=\int_{x_i}^{x_f} p(x)\mathrm{d}x+2\int_{x_f}^{b} p(x)\mathrm{d}x \tag{B.18}$$

Therefore, we have different formulas for even or odd n:

$$n = 2m+2 \implies \int_{x_i}^{x_f} p(x)\,\mathrm{d}x_{(n)} = \int_{x_i}^{x_f} p(x)\mathrm{d}x + 2\int_{x_f}^{b} p(x)\mathrm{d}x + m\Omega(E) \tag{B.19}$$

$$n = 2m+1 \implies \int_{x_i}^{x_f} p(x)\,\mathrm{d}x_{(n)} = \int_{x_i}^{x_f} p(x)\mathrm{d}x + m\Omega(E) \tag{B.20}$$

Before writing the semiclassical fixed energy propagator more explicitly, we should find the number of turning points N_n for the even and odd cases. For the green paths, $N_n = n-1$ by inspection.

$$\begin{aligned} K_{sc}^{\text{green}}(E;x_f,x_i) &= \sum_{m=0}^{\infty} \frac{e^{-i\frac{\pi}{2}(2m+1)}}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\left(\int_{x_i}^{x_f} p(x)\mathrm{d}x + 2\int_{x_f}^{b} p(x)\mathrm{d}x + m\Omega(E)\right)} \quad \text{(even)} \\ &\quad + \sum_{m=0}^{\infty} \frac{e^{-i\frac{\pi}{2}(2m)}}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\left(\int_{x_i}^{x_f} p(x)\mathrm{d}x + m\Omega(E)\right)} \quad \text{(odd)} \qquad \text{(B.21)} \\ &= \frac{e^{-i\frac{\pi}{2}}}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\left(\int_{x_i}^{x_f} p(x)\mathrm{d}x + 2\int_{x_f}^{b} p(x)\mathrm{d}x\right)} \frac{1}{1+e^{\frac{i}{\hbar}\Omega(E)}} \\ &\quad + \frac{1}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\int_{x_i}^{x_f} p(x)\mathrm{d}x} \frac{1}{1+e^{\frac{i}{\hbar}\Omega(E)}}, \qquad \text{(B.22)} \end{aligned}$$

where we used the geometric series as

$$\sum_{m=0}^{\infty} (-1)^m e^{\frac{i}{\hbar}m\Omega(E)} = \frac{1}{1+e^{\frac{i}{\hbar}\Omega(E)}} \tag{B.23}$$

Hence,

$$K_{sc}^{\text{green}}(E;x_f,x_i) = \frac{1}{\sqrt{|v(x_i)v(x_f)|}} \frac{e^{\frac{i}{\hbar}\int_{x_i}^{x_f} p(x)\mathrm{d}x}}{1+e^{\frac{i}{\hbar}\Omega(E)}} \left(1 + e^{-i\frac{\pi}{2}} e^{\frac{2i}{\hbar}\int_{x_f}^{b} p(x)\mathrm{d}x}\right) \tag{B.24}$$

We can perform a similar computation for the pink paths. We have, as for the green path, the recursion relation (B.17), as well as the first 2 integrals:

$$\int_{x_i}^{x_f} p(x)\,\mathrm{d}x_{(1)} = \int_{x_i}^{x_f} p(x)\,\mathrm{d}x + 2\int_{a}^{x_i} p(x)\,\mathrm{d}x \tag{B.25}$$

$$\int_{x_i}^{x_f} p(x)\,\mathrm{d}x_{(2)} = \int_{x_i}^{x_f} p(x)\,\mathrm{d}x + 2\int_{a}^{x_i} p(x)\,\mathrm{d}x + 2\int_{x_f}^{b} p(x)\,\mathrm{d}x \tag{B.26}$$

Therefore, we have

$$n = 2m+2 \implies \int_{x_i}^{x_f} p(x)\,\mathrm{d}x_{(n)} = \int_{x_i}^{x_f} p(x)\,\mathrm{d}x + 2\int_{a}^{x_i} p(x)\,\mathrm{d}x + 2\int_{x_f}^{b} p(x)\,\mathrm{d}x + m\Omega(E)$$

$$n = 2m+1 \implies \int_{x_i}^{x_f} p(x)\,\mathrm{d}x_{(n)} = \int_{x_i}^{x_f} p(x)\,\mathrm{d}x + 2\int_{a}^{x_i} p(x)\,\mathrm{d}x + m\Omega(E)$$

By the same computation as previously (this time $N_n = n$), we find

$$K_{sc}^{\text{pink}}(E;x_f,x_i) = \sum_{m=0}^{\infty} \frac{e^{-i\frac{\pi}{2}(2m+2)}}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\left(\int_{x_i}^{x_f} p(x)\,\mathrm{d}x + 2\int_a^{x_i} p(x)\,\mathrm{d}x + 2\int_{x_f}^{b} p(x)\,\mathrm{d}x + m\Omega(E)\right)} \quad \text{(even)}$$

$$+ \sum_{m=0}^{\infty} \frac{e^{-i\frac{\pi}{2}(2m+1)}}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\left(\int_{x_i}^{x_f} p(x)\,\mathrm{d}x + 2\int_a^{x_i} p(x)\,\mathrm{d}x + m\Omega(E)\right)} \quad \text{(odd)}$$

$$= \frac{-1}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\left(\int_{x_i}^{x_f} p(x)\,\mathrm{d}x + 2\int_a^{x_i} p(x)\,\mathrm{d}x + 2\int_{x_f}^{b} p(x)\,\mathrm{d}x\right)} \frac{1}{1+e^{\frac{i}{\hbar}\Omega(E)}}$$

$$+ \frac{e^{-i\frac{\pi}{2}}}{\sqrt{|v(x_i)v(x_f)|}} e^{\frac{i}{\hbar}\left(\int_{x_i}^{x_f} p(x)\,\mathrm{d}x + 2\int_a^{x_i} p(x)\,\mathrm{d}x\right)} \frac{1}{1+e^{\frac{i}{\hbar}\Omega(E)}} \tag{B.27}$$

Therefore, the pink path contribution to the fixed energy propagator is given by

$$K_{sc}^{\text{pink}}(E;x_f,x_i) = \frac{e^{-i\frac{\pi}{2}}}{\sqrt{|v(x_i)v(x_f)|}} \frac{e^{\frac{i}{\hbar}\left(\int_{x_i}^{x_f} p(x)\,\mathrm{d}x + 2\int_a^{x_i} p(x)\,\mathrm{d}x\right)}}{1+e^{\frac{i}{\hbar}\Omega(E)}} \left(1 + e^{-i\frac{\pi}{2}} e^{\frac{2i}{\hbar}\int_{x_f}^{b} p(x)\mathrm{d}x}\right)$$

This allows us to compute the full fixed energy propagator in the semiclassical approximation:

$$K_{sc}(E;x_f,x_i) = \frac{1}{\sqrt{|v(x_i)v(x_f)|}} \frac{e^{\frac{i}{\hbar}\int_{x_i}^{x_f} p(x)\mathrm{d}x}}{1+e^{\frac{i}{\hbar}\Omega(E)}} \left(1 + e^{-i\frac{\pi}{2}} e^{\frac{2i}{\hbar}\int_{x_f}^{b} p(x)\mathrm{d}x}\right) \left(1 + e^{-i\frac{\pi}{2}} e^{\frac{2i}{\hbar}\int_{a}^{x_i} p(x)\mathrm{d}x}\right)$$

Notice now that we can write

$$\int_{x_i}^{x_f} p(x)\mathrm{d}x = \underbrace{\int_a^b p(x)\mathrm{d}x}_{=\frac{1}{2}\Omega(E)} - \int_a^{x_i} p(x)\mathrm{d}x - \int_{x_f}^{b} p(x)\mathrm{d}x \tag{B.28}$$

which allows us to write

$$K_{sc}(E;x_f,x_i) = \frac{1}{\sqrt{|v(x_i)v(x_f)|}} \frac{e^{\frac{i}{\hbar}\frac{\Omega(E)}{2}}}{1+e^{\frac{i}{\hbar}\Omega(E)}}$$

$$\cdot \left(e^{-\frac{i}{\hbar}\int_{x_f}^{b} p(x)\mathrm{d}x} + e^{-i\frac{\pi}{2}} e^{\frac{i}{\hbar}\int_{x_f}^{b} p(x)\mathrm{d}x}\right) \left(e^{-\frac{i}{\hbar}\int_{a}^{x_i} p(x)\mathrm{d}x} + e^{-i\frac{\pi}{2}} e^{\frac{i}{\hbar}\int_{a}^{x_i} p(x)\mathrm{d}x}\right)$$

$$= \frac{4e^{-i\frac{\pi}{2}} e^{\frac{i}{\hbar}\frac{\Omega(E)}{2}}}{1+e^{\frac{i}{\hbar}\Omega(E)}} \cdot \frac{\cos\left(\frac{1}{\hbar}\int_{x_f}^{b} p(x)\mathrm{d}x - \frac{\pi}{4}\right) \cos\left(\frac{1}{\hbar}\int_{a}^{x_i} p(x)\mathrm{d}x - \frac{\pi}{4}\right)}{\sqrt{|v(x_i)v(x_f)|}} \tag{B.29}$$

In order to understand the analytic structure of this propagator, consider the denominator $1 + e^{\frac{i}{\hbar}\Omega(E)}$. This vanishes when

$$\Omega(E) = \pi\hbar(2n+1) = \left(n + \frac{1}{2}\right) h, \tag{B.30}$$

which is exactly the Bohr-Sommerfeld quantization condition. Our semiclassical propagator now exhibits poles whenever $E = E_n$, where E_n are defined such that $\Omega(E_n) = (n + 1/2)h$. This method therefore allows us to see the discrete structure of the energy levels, unlike the more approximate method from the main text.

Moreover, we can extract the wavefunctions from the residue at the poles. Recall equation (3.31), which tells us that

$$\mathrm{Res}(K(E; x_f, x_i), E = E_n) = i\hbar\psi_n(x_f)\psi_n^*(x_i). \tag{B.31}$$

In order to compute the residues from (B.29), notice that

$$\cos\left(\frac{1}{\hbar}\int_{x_f}^{b} p(x)\mathrm{d}x - \frac{\pi}{4}\right) = \cos\left(\frac{\Omega(E)}{2\hbar} - \frac{1}{\hbar}\int_{a}^{x_f} p(x)\mathrm{d}x - \frac{\pi}{4}\right) \tag{B.32}$$

$$\xrightarrow{E\to E_n} \cos\left(\pi n - \frac{1}{\hbar}\int_{a}^{x_f} p(x)\mathrm{d}x + \frac{\pi}{4}\right) \tag{B.33}$$

$$= (-1)^n \cos\left(\frac{1}{\hbar}\int_{a}^{x_f} p(x)\mathrm{d}x - \frac{\pi}{4}\right) \tag{B.34}$$

Furthermore,

$$1 + e^{\frac{i}{\hbar}\Omega(E)} = \underbrace{1 + e^{\frac{i}{\hbar}\Omega(E_n)}}_{=0} + \frac{i}{\hbar}\frac{\partial\Omega}{\partial E}e^{\frac{i}{\hbar}\Omega(E_n)}(E - E_n) + \mathcal{O}((E - E_n)^2) \tag{B.35}$$

$$= -\frac{i}{\hbar}\frac{\partial\Omega}{\partial E}(E - E_n) + \mathcal{O}((E - E_n)^2) \tag{B.36}$$

Now $\frac{\partial\Omega}{\partial E}$ can be computed as follows:

$$\frac{\partial\Omega}{\partial E} = 2\frac{\partial}{\partial E}\int_a^b \sqrt{2m(E - V(x))}\mathrm{d}x \tag{B.37}$$

$$= 2\frac{\partial b}{\partial E}p(b) - 2\frac{\partial a}{\partial E}p(a) + 2\int_a^b \frac{\mathrm{d}x}{v(x)} \tag{B.38}$$

$$= T, \tag{B.39}$$

where we used the fact that $p(a) = p(b) = 0$ by definition of the turning points, and we defined T to be the period of trajectories with energy E. Therefore,

$$\frac{1}{1 + e^{\frac{i}{\hbar}\Omega(E)}} \xrightarrow{E\to E_n} \frac{i\hbar}{T(E - E_n)} \tag{B.40}$$

and we can write

$$K_{sc}(E; x_f, x_i) \xrightarrow{E\to E_n} 4e^{i\pi n}\frac{i\hbar}{T(E - E_n)} \cdot \frac{(-1)^n \cos\left(\frac{1}{\hbar}\int_a^{x_f} p(x)\mathrm{d}x - \frac{\pi}{4}\right)\cos\left(\frac{1}{\hbar}\int_a^{x_i} p(x)\mathrm{d}x - \frac{\pi}{4}\right)}{\sqrt{|v(x_i)v(x_f)|}}$$

$$= \frac{i\hbar}{E - E_n}\frac{2\cos\left(\frac{1}{\hbar}\int_a^{x_f} p(x)\mathrm{d}x - \frac{\pi}{4}\right)}{\sqrt{|v(x_f)T|}}\frac{2\cos\left(\frac{1}{\hbar}\int_a^{x_i} p(x)\mathrm{d}x - \frac{\pi}{4}\right)}{\sqrt{|v(x_i)T|}} \tag{B.41}$$

We can therefore read off the wavefunctions!

$$\mathrm{Res}(K_{sc}(E;x_f,x_i),E=E_n) = i\hbar\psi_n^{\mathrm{WKB}}(x_f)\psi_n^{*,\mathrm{WKB}}(x_i), \tag{B.42}$$

$$\text{where } \psi_n^{\mathrm{WKB}}(x) = \frac{2}{\sqrt{|v(x)T|}}\cos\left(\frac{1}{\hbar}\int_a^x p(x)\mathrm{d}x - \frac{\pi}{4}\right) \tag{B.43}$$

This corresponds to the usual WKB wavefunctions obtained from the Schrödinger equation.

As a last comment, note that these wavefunctions are already normalized:

$$\int_{-\infty}^{\infty}\mathrm{d}x\,|\psi_n^{\mathrm{WKB}}(x)|^2 \approx \int_a^b \mathrm{d}x\,\frac{4}{|v(x)T|}\cos^2\left(\frac{1}{\hbar}\int_a^x p(x)\mathrm{d}x - \frac{\pi}{4}\right), \tag{B.44}$$

where we approximate the integration over the real numbers by the integration between the turning points since the WKB wavefunction is exponentially decaying outside the classically allowed region. Furthermore, the cosine in the integrand oscillates very fast since we are considering the semiclassical limit where "$p \gg \hbar$". We can therefore approximate $\cos^2$ by $\frac{1}{2}$, which leads to the desired normalization:

$$\int_{-\infty}^{\infty}\mathrm{d}x\,|\psi_n^{\mathrm{WKB}}(x)|^2 \approx \frac{1}{T}\int_a^b \mathrm{d}x\,\frac{2}{|v(x)|} = 1, \tag{B.45}$$

since $v(x) > 0$ between a and b and $T = 2\int_a^b \mathrm{d}t$.

B.5 The instanton prefactor

The goal of this section is to compute the prefactor R that appeared in lecture 10.

First, we introduce the **twisted partition function** Z_a:

$$Z_a[\beta] = \mathrm{Tr}\left(\hat{P}e^{-\frac{\beta}{\hbar}\hat{H}}\right), \tag{B.46}$$

where $\hat{P}$ is the operator that sends $x \to -x$, and $_a$ stands for "anti-periodic". Computing the trace in the complete basis of energy eigenstates, we have

$$Z_a[\beta] = \sum_n \langle n|\, \hat{P}\, |n\rangle\, e^{-\frac{\beta}{\hbar}E_n} \tag{B.47}$$

Now we know that

$$\hat{P}\,|n\rangle = \begin{cases} +\,|n\rangle\,, & n = \text{even} \\ -\,|n\rangle\,, & n = \text{odd} \end{cases}, \tag{B.48}$$

simply because $\psi_n(x) = \psi_n(-x)$ for even n and $\psi_n(x) = -\psi_n(-x)$ for odd n. Therefore,

$$Z_a[\beta] = \sum_n (-1)^n e^{-\frac{\beta}{\hbar}E_n} \tag{B.49}$$

Let us now consider the range of β for which a single instanton dominates:

$$\beta\omega \gg 1 \quad \text{and} \quad \frac{\beta}{\hbar}(E_1 - E_0) \ll 1 \tag{B.50}$$

We can then write the twisted partition function as

$$Z_a[\beta] = e^{-\frac{\beta}{\hbar}E_0}\left(1 - e^{-\frac{\beta}{\hbar}(E_1-E_0)} + e^{-\frac{\beta}{\hbar}(E_2-E_0)} + \dots\right) \tag{B.51}$$

$$\approx e^{-\frac{\beta}{\hbar}E_0}\left(\frac{\beta}{\hbar}(E_1 - E_0)\right) \tag{B.52}$$

where we used both assumptions from (B.50), as well as the fact that $E_k - E_0 \sim \hbar\omega$ for $k \geq 2$ (the non-perturbative splitting only occurs between E_1 and E_0, the others are computed using usual HO perturbative arguments). Since $E_k - E_0 \sim \hbar\omega$, all the terms in $\dots$ are exponentially suppressed in the $\beta\omega \gg 1$ limit.

Finally, we can write $E_0 = \frac{\hbar\omega}{2}$ up to $\mathcal{O}(\lambda)$:

$$Z_a[\beta] \approx e^{-\frac{\beta\omega}{2}}\frac{\beta}{\hbar}(E_1 - E_0) \tag{B.53}$$

The reason why the twisted partition function is useful is because in the limit (B.50), it is proportional to the energy splitting $E_1 - E_0$. Note that this result was obtained after making two approximations: the $\beta\omega \gg 1$ approximation to drop the terms in (B.51),

and the leading order in λ to write equation (B.53).

In these limits, one can refine the result above by using the harmonic oscillator twisted partition function. Indeed,

$$Z_a^{\mathrm{HO}}[\beta] = \sum_n (-1)^n e^{-\beta\omega(n+1/2)} \xrightarrow{\beta\omega\gg 1} e^{-\frac{\beta\omega}{2}} + \dots, \tag{B.54}$$

which means that

$$\frac{Z_a[\beta]}{Z_a^{\mathrm{HO}}[\beta]} \to \frac{\beta}{\hbar}(E_1 - E_0) \tag{B.55}$$

in the limits $\beta\omega \gg 1$ and $\frac{\beta}{\hbar}(E_1 - E_0) \ll 1$.

Path integral representation of Z_a
Using the definition of Z_a, but evaluating the trace in the position basis, we find

$$Z_a[\beta] = \mathrm{Tr}\left(\hat{P}e^{-\frac{\beta}{\hbar}\hat{H}}\right) = \int \mathrm{d}x \, \langle x| \, \hat{P}e^{-\frac{\beta}{\hbar}\hat{H}} \, |x\rangle \tag{B.56}$$

$$= \int \mathrm{d}x \, \langle -x| \, e^{-\frac{\beta}{\hbar}\hat{H}} \, |x\rangle = \int \mathrm{d}x \, K_E(-x, x; \beta) \tag{B.57}$$

$$= \int_{x(\tau+\beta)=-x(\tau)} \mathcal{D}[x] e^{-\frac{1}{\hbar}S_E[x]} \tag{B.58}$$

The boundary conditions are antiperiodic: $x(\tau + \beta) = -x(\tau)$, which is where the name "twisted" partition function comes from. We can now perform the saddle point approximation, where the saddles are paths verifying the Euclidean equation of motion

$$\frac{\delta S_E}{\delta x} = 0 \Leftrightarrow m\ddot{x} = V'(x), \tag{B.59}$$

which is simply classical motion in the inverted potential. The main difference is that now the boundary conditions are antiperiodic, which is equivalent to periodic BC over the interval 2β:

$$x(\tau + \beta) = -x(\tau) \implies x(\tau + 2\beta) = -x(\tau + \beta) = x(\tau) \tag{B.60}$$

For a given energy $E < 0$, there are classical turning points in the inverted potential at $\pm x(E)$ (with $0 < x(E) < a$). Paths with this energy oscillate between the turning points with period $T(E)$, which means that

$$\beta = \left(\frac{1}{2} + n\right) T(E), \quad n = 0, 1, 2, \dots \tag{B.61}$$

Indeed, one can add any integer periods to β and still verify the anti-periodic BC. At this level, we have multi-instanton solutions, since there are many paths in this potential with these boundary conditions. However, in the regime (B.50), the $n = 0$ path dominates.

Euclidean action

Consider first the expression of β with the period written explicitly:

$$\beta = \left(\frac{1}{2}+n\right) 2\int_{-x(E)}^{x(E)} \frac{\mathrm{d}x}{\dot{x}} = \left(\frac{1}{2}+n\right)\int_{-x(E)}^{x(E)} \mathrm{d}x \sqrt{\frac{2m}{E+V(x)}}, \tag{B.62}$$

where we used $E = \frac{1}{2}m\dot{x}^2 - V(x) = \text{const}$. We can then use this to find a convenient expression for the Euclidean action:

$$S_E = \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \,\frac{1}{2}m\dot{x}^2 + V(x) = \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\,(m\dot{x}^2 - E) \tag{B.63}$$

$$= -\beta E + \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, \dot{x}\sqrt{2m(E+V(x))} \tag{B.64}$$

Note now that we can convert the integral over τ to an integral over x, but we have to be careful about the sign of $\dot{x}$. Indeed, for $n > 1$, β corresponds to multiple half periods. For example, $n = 1$ corresponds to 3 half periods, so we can write

$$S_E = -\beta E + (2n+1)\int_{-x(E)}^{x(E)} \mathrm{d}x\,\sqrt{2m(E+V(x))} \tag{B.65}$$

Using the explicit expression for β from (B.62), we find

$$S_E = \left(\frac{1}{2}+n\right)\left[-E\int_{-x(E)}^{x(E)} \mathrm{d}x\sqrt{\frac{2m}{E+V(x)}} + 2\int_{-x(E)}^{x(E)} \mathrm{d}x\,\sqrt{2m(E+V(x))}\right] \tag{B.66}$$

In the limit $\beta \gg \frac{1}{\omega}$, we are equivalently interested at large periods of oscillations, i.e. the limit $E \to 0^-$. In that limit, the turning points become $\pm a$ and

$$S_E \approx (2n+1)\int_{-a}^{a} \mathrm{d}x\,\sqrt{2mV(x)} \equiv (2n+1)S_I, \tag{B.67}$$

where we used the definition of S_I (eq. 3.152).

The zero mode

We want to evaluate the exponential in the Euclidean path integral on the classical trajectory, with some small perturbation. To quadratic order,

$$\frac{1}{\hbar}S_E\left[x_c + \sqrt{\frac{\hbar}{m}}y\right] \approx \frac{1}{\hbar}S_E[x_c] + \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \frac{1}{2}\dot{y}^2 + \frac{1}{2m}V''(x_c)y^2 \tag{B.68}$$

$$\approx \frac{1}{\hbar}S_E[x_c] + \frac{1}{2}\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \mathrm{d}\tau_2\, y(\tau_1)\mathcal{O}(\tau_1,\tau_2)y(\tau_2),$$

where

$$\mathcal{O}(\tau_1,\tau_2) = \delta(\tau_1-\tau_2)\left(-\frac{\mathrm{d}^2}{\mathrm{d}\tau_2^2} + \frac{1}{m}V''(x_c(\tau_2))\right). \tag{B.69}$$

Before plugging this result into the path integral, we should think about what are the classical solutions we should consider when performing the saddle point approximation. It turns out that both the instanton and the anti-instanton verify $x(\tau+\beta) = -x(\tau)$. Therefore, when using the saddle point approximation we should add a factor of 2 to account for the 2 distinct classical solutions: the twisted partition function can be approximated as

$$Z_a[\beta] = \int_{x(\tau+\beta)=-x(\tau)} \mathcal{D}[x] e^{-\frac{1}{\hbar}S_E[x]} \tag{B.70}$$

$$\approx 2e^{-\frac{1}{\hbar}S_I} \int_{y(\tau+\beta)=-y(\tau)} \mathcal{D}[x] e^{-\frac{1}{2}y\cdot\mathcal{O}\cdot y}, \tag{B.71}$$

where we now write $S_E[x_c] = S_I$ for simplicity since the action for both classical paths (the instanton and anti-instanton) are the same. Schematically, the path integral over y can be related to the **determinant** of $\mathcal{O}$, up to some normalization $\mathcal{N}$:

$$Z_a[\beta] \approx 2e^{-\frac{1}{\hbar}S_I} \mathcal{N} (\det{}_a \mathcal{O})^{-1/2}, \tag{B.72}$$

where by $\det_a$ we denote the determinant over antiperiodic paths.

The first problem we encounter is that this determinant is formally 0. This is because $\mathcal{O}$ has a **zero mode** (a zero eigenvalue). Indeed, if we take the derivative of the Euclidean EOM, we find that $\dot{x}_c(\tau)$ is an eigenfunction of $\mathcal{O}$ with eigenvalue 0:

$$m\ddot{x}_c = V'(x_c) \implies m\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\dot{x}_c = V''(x_c)\dot{x}_c \implies \mathcal{O}\cdot\dot{x}_c(\tau) = 0, \tag{B.73}$$

where we used the definition of $\mathcal{O}$:

$$\mathcal{O} = -\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + \frac{1}{m}V''(x_c(\tau)) \tag{B.74}$$

What to do now? Let us decompose $y(\tau)$ in eigenfunctions y_n of $\mathcal{O}$. These functions verify the following relations

$$\mathcal{O}\cdot y_n(\tau) = \lambda_n y_n(\tau), \quad y_n(\tau+\beta) = -y_n(\tau) \tag{B.75}$$

$$\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, y_n(\tau) y_m(\tau) = \delta_{nm} \tag{B.76}$$

We can now use these eigenfunctions to write

$$x(\tau) = x_c(\tau) + \sqrt{\frac{\hbar}{m}} \sum_{n=0}^{\infty} c_n y_n(\tau). \tag{B.77}$$

We know that there must be a mode proportional to $\dot{x}_c(\tau)$, which we call the zero mode. Without loss of generality, we set

$$y_0(\tau) \equiv A\dot{x}_c(\tau), \tag{B.78}$$

where now $\lambda_0 = 0$. We can determine A by enforcing normalization:

$$1 = \int_{-\beta/2}^{\beta/2} y_0(\tau)^2 = A^2 \int_{-\beta/2}^{\beta/2} \dot{x}_c^2 \tag{B.79}$$

$$= A^2 \int_{-x(E)}^{x(E)} \mathrm{d}x \sqrt{\frac{2(V(x)+E)}{m}} \xrightarrow{E\to 0^-} A^2 \frac{S_I}{m}, \tag{B.80}$$

where S_I was defined in equation (3.152). Therefore, $A \equiv \sqrt{\frac{m}{S_I}}$. In this basis, we find

$$Z_a[\beta] \approx 2e^{-\frac{1}{\hbar}S_I} \int_{y(\tau+\beta)=-y(\tau)} \mathcal{D}[x] e^{-y\cdot\mathcal{O}\cdot y} \tag{B.81}$$

$$\approx 2e^{-\frac{1}{\hbar}S_I} \mathcal{N} \int \prod_{n=0}^{\infty} \frac{\mathrm{d}c_n}{\sqrt{2\pi}} e^{-\frac{1}{2}\lambda_n c_n^2} \tag{B.82}$$

One can now see that the c_0 integral will diverge since there is no c_0 appearing in the exponent ($\lambda_0 = 0$). However, we have isolated the problematic piece and can now write

$$Z_a[\beta] \approx 2e^{-\frac{1}{\hbar}S_I} \int \frac{\mathrm{d}c_0}{\sqrt{2\pi}} \mathcal{N} \left(\prod_{n=1}^{\infty} \lambda_n \right)^{-1/2} \tag{B.83}$$

We now define the following determinant:

$$\det{}'_a \mathcal{O} \equiv \prod_{n=1}^{\infty} \lambda_n, \tag{B.84}$$

where the prime means that the zero-mode was removed from the product of eigenvalues. This determinant can be expressed as a derivative of a deformed determinant:

$$\det{}'_a \mathcal{O} = \partial_\theta \det{}_a(\mathcal{O}+\theta)|_{\theta=0} \tag{B.85}$$

Indeed, the eigenvalues of $\mathcal{O}+\theta$ are simply $\lambda_n + \theta$, so

$$\det{}_a(\mathcal{O}+\theta) = \prod_{n=0}^{\infty} (\lambda_n + \theta) \tag{B.86}$$

$$= \underbrace{\prod_{n=0}^{\infty} \lambda_n}_{=0} + \theta \prod_{n=1}^{\infty} \lambda_n + \mathcal{O}(\theta^2), \tag{B.87}$$

which directly proves (B.85).

Now, we should understand how to deal with the integral over c_0. To do so, we can think of another way to express $x(\tau)$ in terms of x_c and y_n's. We can write

$$x(\tau) = x_c(\tau + \tau_0) + \sqrt{\frac{\hbar}{m}} \sum_{n=1}^{\infty} c_n y_n(\tau), \tag{B.88}$$

where now τ_0 is a new variable of integration which "replaces" the old variable c_0. From an infinitesimal point of view, this is sensible as for small τ_0, we have $x_c(\tau+\tau_0) \approx x_c(\tau) + \dot{x}_c(\tau)\tau_0$, and we know that y_0 is proportional to $\dot{x}_c$. More explicitly, upon varying the parameters τ_0 and c_k in equations (B.77) and (B.88) we find

$$\delta x(\tau) = \sqrt{\frac{\hbar}{m}} \sum_{n=0}^{\infty} \delta c_n y_n(\tau) \tag{B.89}$$

$$\text{and } \delta x(\tau) = \delta\tau_0 \dot{x}_c(\tau) + \sqrt{\frac{\hbar}{m}} \sum_{n=0}^{\infty} \delta c_n y_n(\tau). \tag{B.90}$$

We can therefore identify

$$\delta c_0 = \sqrt{\frac{S_I}{\hbar}} \delta\tau_0, \tag{B.91}$$

where we used $A \equiv \sqrt{\frac{m}{S_I}}$. The integral over c_0 can now be understood!

$$\int \frac{\mathrm{d}c_0}{\sqrt{2\pi}} = \sqrt{\frac{S_I}{2\pi\hbar}} \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_0 = \sqrt{\frac{S_I}{2\pi\hbar}}\beta, \tag{B.92}$$

and therefore

$$Z_a[\beta] = 2e^{-\frac{1}{\hbar}S_I} \sqrt{\frac{S_I}{2\pi\hbar}} \beta \mathcal{N} \left(\frac{\partial}{\partial\theta} \det{}_a(\mathcal{O}+\theta)\Big|_{\theta=0} \right)^{-1/2} \tag{B.93}$$

More practically, we saw that the zero modes are related to the positions of the instanton (τ_0), and that (B.88) was a better parametrization than our naive first guess. Instead of a strange integral over c_0, we obtained an integral over the position of the instanton, which has a finite range.

Removing $\mathcal{N}$ with the help of our friend the harmonic oscillator

Since the action of the harmonic oscillator is already gaussian, we can simply write

$$Z_a^{\mathrm{HO}}[\beta] = \int_{x(\tau+\beta)=-x(\tau)} \mathcal{D}[x] e^{-\frac{1}{\hbar}S_E[x]} = \int_{y(\tau+\beta)=-y(\tau)} \mathcal{D}[y] e^{-\frac{1}{2}y\cdot\mathcal{O}_{\mathrm{HO}}\cdot y} \tag{B.94}$$

$$= \mathcal{N} \left(\det{}_a \mathcal{O}_{\mathrm{HO}}\right)^{-1/2}, \tag{B.95}$$

where we used $x = \sqrt{\frac{\hbar}{m}} y$ as before and we defined

$$\mathcal{O}_{\mathrm{HO}} = -\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + \omega^2. \tag{B.96}$$

Note that this operator is exactly what we would have found using equation (B.74) with $V(x) = \frac{1}{2}m\omega^2 x^2$. Therefore, we have

$$\frac{Z_a[\beta]}{Z_a^{\mathrm{HO}}[\beta]} = 2e^{-\frac{1}{\hbar}S_I} \sqrt{\frac{S_I}{2\pi\hbar}} \beta \left(\frac{\partial}{\partial\theta} \frac{\det{}_a(\mathcal{O}+\theta)}{\det{}_a(\mathcal{O}_{\mathrm{HO}})}\Big|_{\theta=0} \right)^{-1/2}, \tag{B.97}$$

where the operators $\mathcal{O}$ and $\mathcal{O}_{\text{HO}}$ were defined in equations (B.96) and (B.74) Comparing this expression with equation (B.55), we have an expression for the energy splitting!

$$\boxed{E_1 - E_0 = 2\hbar e^{-\frac{1}{\hbar}S_I}\sqrt{\frac{S_I}{2\pi\hbar}}\left(\frac{\partial}{\partial\theta}\frac{\det_a(\mathcal{O}+\theta)}{\det_a(\mathcal{O}_{\text{HO}})}\bigg|_{\theta=0}\right)^{-1/2}} \tag{B.98}$$

In the lecture, we had defined some temporary variable R to account for the prefactor. Here, we can compare with the result from the lecture (3.180) to obtain an expression for R:

$$R \equiv \sqrt{\frac{S_I}{2\pi\hbar}}\left(\frac{\partial}{\partial\theta}\frac{\det_a(\mathcal{O}+\theta)}{\det_a(\mathcal{O}_{\text{HO}})}\bigg|_{\theta=0}\right)^{-1/2} \tag{B.99}$$

In order to compute these determinants, we will need to use a formalism similar to the one developed in Lecture 3 with the Gelfand-Yaglom formula. The antiperiodic boundary conditions require us to modify the argument, which is presented below.

Gelfand-Yaglom reloaded
We are interested in the eigenvalue equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + W(\tau)\right]\psi(\tau) = \lambda\psi(\tau), \quad \psi(\tau+\beta) = -\psi(\tau), \tag{B.100}$$

where W now plays the role of $V''(x_c(\tau))$. Consider now 2 linearly independent solutions $\psi_{1,2}(\tau)$. Define then the matrix $M_\lambda(\tau)$ as

$$M_\lambda(\tau) \equiv \begin{pmatrix}\psi_1(\tau) & \psi_2(\tau)\\ \dot\psi_1(\tau) & \dot\psi_2(\tau)\end{pmatrix}, \quad \text{with initial condition} \quad M_\lambda(-\beta/2) = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \tag{B.101}$$

The subscript λ is present because the functions ψ_1 and ψ_2 solve the differential equation that depends on λ.

The determinant of $M(\tau)$ is the Wronskian, which is constant in time. Therefore, evaluating it at $\tau = -\beta/2$ we find

$$\det M_\lambda(\tau) = 1, \ \forall\tau \tag{B.102}$$

Now we know that the most general solution to equation (B.100) can be written as a linear combination of ψ_1 and ψ_2 with constant coefficients:

$$\psi(\tau) = A\psi_1(\tau) + B\psi_2(\tau) \tag{B.103}$$
$$\dot\psi(\tau) = A\dot\psi_1(\tau) + B\dot\psi_2(\tau) \tag{B.104}$$

Evaluating at $\tau = -\beta/2$ leads to an expression of A and B in terms of the initial conditions of ψ:

$$\psi(-\beta/2) = A, \quad \dot\psi(-\beta/2) = B \tag{B.105}$$

Therefore,

$$\begin{pmatrix}\psi(\tau)\\ \dot{\psi}(\tau)\end{pmatrix} = M_\lambda(\tau)\begin{pmatrix}\psi(-\beta/2)\\ \dot{\psi}(-\beta/2)\end{pmatrix} \tag{B.106}$$

If λ is an eigenvalue of $\mathcal{O}$, then ψ is an antiperiodic solution of (B.100) and we can therefore write

$$(M_\lambda(\beta/2)+\mathbb{1})\begin{pmatrix}\psi(-\beta/2)\\ \dot{\psi}(-\beta/2)\end{pmatrix} = 0 \tag{B.107}$$

This tells us that the matrix $M_\lambda(\beta/2)+\mathbb{1}$ is not invertible, or equivalently that it has vanishing determinant. This condition is very useful:

$$0 = \det(M_\lambda(\beta/2)+\mathbb{1}) = \det\begin{pmatrix}\psi_1(\beta/2)+1 & \psi_2(\beta/2)\\ \dot{\psi}_1(\beta/2) & \dot{\psi}_2(\beta/2)+1\end{pmatrix} \tag{B.108}$$

$$= \det M_\lambda(\beta/2) + \operatorname{Tr} M_\lambda(\beta/2) + 1, \tag{B.109}$$

where the determinant of the 2×2 matrix was computed explicitly. Now we know that $\det M_\lambda(\beta/2)$, so we obtain

$$\operatorname{Tr}\left[M_\lambda(\beta/2)+\mathbb{1}\right] = 0 \tag{B.110}$$

This has significant consequences for our computation. We claim that

$$\frac{\det\left[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+W(\tau)-\lambda\right]}{\det\left[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+\tilde{W}(\tau)-\lambda\right]} = \frac{\operatorname{Tr}\left[M_\lambda(\beta/2)+\mathbb{1}\right]}{\operatorname{Tr}\left[\tilde{M}_\lambda(\beta/2)+\mathbb{1}\right]}. \tag{B.111}$$

In order to justify this claim, we invoke the following mathematical result: if two complex functions have the same zeroes and poles, and the same asymptotic behavior as $|z|\to\infty$, then they are the same function.

Using this result, we can think of the left and right-hand side above as complex functions of $\lambda\in\mathbb{C}$ and compare their properties:

- Zeroes: when λ is an eigenvalue of $\mathcal{O} = -\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+W(\tau)$, both sides vanish.
- Poles: when λ is an eigenvalue of $\tilde{\mathcal{O}} = -\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+\tilde{W}(\tau)$, both sides have a pole.
- Asymptotic behavior: as $\lambda\to\infty$, both sides tend to 1.

Our claim is therefore verified.

Back to business
The goal is to determine

$$\frac{\partial}{\partial\theta}\frac{\det_a(\mathcal{O}+\theta)}{\det_a(\mathcal{O}_{\mathrm{HO}})}\bigg|_{\theta=0}. \tag{B.112}$$

Using equation (B.111) with $\lambda = 0$, $W(\tau) = V''(x_c(\tau)) + \theta$ and $\tilde{W}(\tau) = \omega^2$, we find

$$\frac{\partial}{\partial\theta}\frac{\det_a(\mathcal{O}+\theta)}{\det_a(\mathcal{O}_{\mathrm{HO}})}\bigg|_{\theta=0} = \frac{\partial}{\partial\theta}\frac{\psi_1^\theta(\beta/2)+\dot{\psi}_2^\theta(\beta/2)+2}{\psi_1^{\mathrm{HO}}(\beta/2)+\dot{\psi}_2^{\mathrm{HO}}(\beta/2)+2}\bigg|_{\theta=0} \tag{B.113}$$

Computing the denominator: we want to solve the equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+\omega^2\right]\psi^{\mathrm{HO}}(\tau) = 0 \implies \psi^{\mathrm{HO}}(\tau) = Ae^{\omega\tau}+Be^{-\omega\tau} \tag{B.114}$$

The initial conditions on ψ_1 and ψ_2 are:

$$\begin{cases}\psi_1(-\beta/2)=1\\ \dot{\psi}_1(-\beta/2)=0\end{cases} \quad\text{and}\quad \begin{cases}\psi_2(-\beta/2)=0\\ \dot{\psi}_2(-\beta/2)=1\end{cases} \tag{B.115}$$

Therefore,

$$\begin{cases}A_1e^{-\omega\beta/2}+B_1e^{\omega\beta/2}=1\\ A_1e^{-\omega\beta/2}-B_1e^{\omega\beta/2}=0\end{cases} \implies \psi_1(\tau)=\cosh(\omega(\tau+\beta/2))$$

$$\begin{cases}A_2e^{-\omega\beta/2}+B_2e^{\omega\beta/2}=0\\ A_2e^{-\omega\beta/2}-B_2e^{\omega\beta/2}=\dfrac{1}{\omega}\end{cases} \implies \psi_2(\tau)=\frac{1}{\omega}\sinh(\omega(\tau+\beta/2))$$

The denominator therefore reads

$$\psi_1^{\mathrm{HO}}(\beta/2)+\dot{\psi}_2^{\mathrm{HO}}(\beta/2)+2 = 2\cosh(\omega\beta))+2 \xrightarrow{\omega\beta\gg1} e^{\omega\beta} \tag{B.116}$$

Computing the numerator: we want to solve the equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+V''(x_c(\tau))+\theta\right]\psi^\theta(\tau) = 0 \tag{B.117}$$

with initial conditions given by (B.115). At first glance, this is a difficult problem. However, we only need to know $\psi_{1,2}$ to leading order in θ since we want to take one derivative and then set θ to 0. At $\theta = 0$, we already have a solution: $\dot{x}_c$ (see B.73). Using the usual Wronskian trick, we can find an independent solution (still for $\theta = 0$), and we can then treat the problem as a **perturbative problem** in θ.

Consider then first the case $\theta = 0$. We know that a solution of the differential equation (B.117) is $\dot{x}_c(\tau)$. Therefore,

$$\psi_1^{(0)}(\tau) \equiv \frac{\dot{x}_c(\tau)}{\dot{x}_c(-\beta/2)} \tag{B.118}$$

In order to see that $\dot{\psi}_1^{(0)}(-\beta/2) = 0$, it is good to turn back to the physics and use our intuition. Since we want $\psi_1^{(0)}$ to be antiperiodic, we should **choose** an energy E such that $\dot{x}_c(\tau)$ has a period $T(E) = 2\beta$.

We then consider paths $x_c(\tau)$ which start at $-\beta/2$ at $x = 0$, go to the turning point of maximal x at $\tau = 0$, and fall back to $x = 0$ at $\beta/2$. These paths are well defined classical solutions which have the correct anti-periodic behaviour. It is now straightforward to see that at $-\beta/2$, x_c has maximum velocity, and therefore $\ddot{x}_c(-\beta/2) = 0$, which trivially implies that $\dot{\psi}_1^{(0)}(-\beta/2) = 0$. Furthermore, we see that since $x_c(\tau)$ is even, $\psi_1^{(0)}(\tau)$ is an odd function:

$$\psi_1^{(0)}(\tau) = -\psi_1^{(0)}(-\tau) \tag{B.119}$$

To summarize, we construct $\psi_1^{(0)}(\tau)$ in terms of a classical path $x_c(\tau)$ which verifies $x_c(-\beta/2) = x_c(\beta/2) = 0$, so that $\psi_1^{(0)}$ solves the differential equation and has the correct initial conditions. Now we also need $\psi_2^{(0)}(\tau)$, but we can obtain it easily using the usual Wronskian formalism:

$$\psi_1\dot{\psi}_2 - \psi_2\dot{\psi}_1 = 1 \implies \frac{\mathrm{d}}{\mathrm{d}\tau}\frac{\psi_2}{\psi_1} = \frac{1}{\psi_1^2(\tau)} \implies \boxed{\psi_2(\tau) = \psi_1(\tau)\int_{-\beta/2}^{\tau}\frac{\mathrm{d}\tau'}{\psi_1^2(\tau')}} \tag{B.120}$$

We now want to go to first order in θ, i.e. we want to find the functions $\psi_{1,2}^{(1)}(\tau)$ that appear in the following expansion:

$$\psi_{1,2}^{\theta}(\tau) = \psi_{1,2}^{(0)}(\tau) + \theta\psi_{1,2}^{(1)}(\tau) + \mathcal{O}(\theta^2) \tag{B.121}$$

Although it is hard to guess a solution for $\psi_{1,2}^{(1)}(\tau)$, it is easy to verify whether a given expression works by plugging it into (B.117).

Exercise B.1 (Verifying the perturbative solution)**.**
Verify that

$$\psi_{1,2}^{\theta}(\tau) = \psi_{1,2}^{(0)}(\tau) + \theta\psi_{1,2}^{(1)}(\tau) + \mathcal{O}(\theta^2) \tag{B.122}$$

with

$$\psi_{1,2}^{(1)}(\tau) = \int_{-\beta/2}^{\tau} d\tau' \left[\psi_2^{(0)}(\tau)\psi_1^{(0)}(\tau') - \psi_1^{(0)}(\tau)\psi_2^{(0)}(\tau')\right]\psi_{1,2}^{(0)}(\tau') \tag{B.123}$$

verifies the differential equation (B.117) to first order in θ.

Equation (B.123) then leads to

$$\frac{\partial}{\partial\theta}\frac{\det_a(\mathcal{O}+\theta)}{\det_a(\mathcal{O}_{\mathrm{HO}})}\bigg|_{\theta=0} = e^{-\omega\beta}\left(\psi_1^{(1)}(\beta/2) + \dot{\psi}_2^{(1)}(\beta/2)\right) \tag{B.124}$$

Computing $\psi_1^{(1)}$ and $\dot{\psi}_2^{(1)}$ at $\beta/2$

We can compute

$$\psi_1^{(1)}(\beta/2) = \int_{-\beta/2}^{\tau} \mathrm{d}\tau' \left[\psi_2^{(0)}(\beta/2)\psi_1^{(0)}(\tau') + \psi_2^{(0)}(\tau')\right] \psi_1^{(0)}(\tau'), \tag{B.125}$$

where we used the oddness of $\psi_1^{(0)}$ (B.119) to obtain $\psi_1^{(0)}(\beta/2) = -1$. Then, notice that

$$\begin{aligned}\dot{\psi}_2^{(1)}(\tau) &= \frac{\mathrm{d}}{\mathrm{d}\tau}\int_{-\beta/2}^{\tau} \mathrm{d}\tau' \left[\psi_2^{(0)}(\tau)\psi_1^{(0)}(\tau') - \psi_1^{(0)}(\tau)\psi_2^{(0)}(\tau')\right] \psi_2^{(0)}(\tau') &\text{(B.126)}\\ &= \underbrace{\left[\psi_2^{(0)}(\tau)\psi_1^{(0)}(\tau) - \psi_1^{(0)}(\tau)\psi_2^{(0)}(\tau)\right]}_{=0} \psi_2^{(0)}(\tau) \\ &\qquad + \int_{-\beta/2}^{\tau} \mathrm{d}\tau' \left[\dot{\psi}_2^{(0)}(\tau)\psi_1^{(0)}(\tau') - \dot{\psi}_1^{(0)}(\tau)\psi_2^{(0)}(\tau')\right] \psi_2^{(0)}(\tau') &\text{(B.127)}\end{aligned}$$

which implies

$$\dot{\psi}_2^{(1)}(\beta/2) = \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau' \left[\dot{\psi}_2^{(0)}(\beta/2)\psi_1^{(0)}(\tau') - \underbrace{\dot{\psi}_1^{(0)}(\beta/2)}_{=0} \psi_2^{(0)}(\tau')\right] \psi_2^{(0)}(\tau') \tag{B.128}$$

In order to compute $\dot{\psi}_2^{(0)}(\beta/2)$, we use the definition (B.120):

$$\begin{aligned}\dot{\psi}_2(\tau) &= \frac{1}{\psi_1(\tau)} + \dot{\psi}_1(\tau)\int_{-\beta/2}^{\tau} \frac{\mathrm{d}\tau'}{\psi_1^2(\tau')} &\text{(B.129)}\\ \implies \dot{\psi}_2(\beta/2) &= -1 &\text{(B.130)}\end{aligned}$$

Therefore, we have

$$\begin{aligned}\psi_1^{(1)}(\beta/2) &= \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau' \left[\psi_2^{(0)}(\beta/2)\psi_1^{(0)}(\tau') + \psi_2^{(0)}(\tau')\right] \psi_1^{(0)}(\tau'), &\text{(B.131)}\\ \dot{\psi}_2^{(1)}(\beta/2) &= \int_{-\beta/2}^{\tau} \mathrm{d}\tau' \left[-\psi_1^{(0)}(\tau')\right] \psi_2^{(0)}(\tau') &\text{(B.132)}\end{aligned}$$

which implies finally that

$$\boxed{\left.\frac{\partial}{\partial\theta}\frac{\det_a(\mathcal{O}+\theta)}{\det_a(\mathcal{O}_{\mathrm{HO}})}\right|_{\theta=0} = e^{-\omega\beta}\psi_2^{(0)}(\beta/2)\int_{-\beta/2}^{\beta/2}\mathrm{d}\tau'\left[\psi_1^{(0)}(\tau')\right]^2} \tag{B.133}$$

We can however simplify this further. First, notice that in the limit $E \to 0_-$,

$$S_c = \int_{-\beta/2}^{\beta/2}\mathrm{d}\tau\left[\frac{1}{2}m\dot{x}_c^2 + V(x_c)\right] = \int_{-\beta/2}^{\beta/2}\mathrm{d}\tau\left[m\dot{x}_c^2 - E\right] \xrightarrow{E\to 0_-} = m\int_{-\beta/2}^{\beta/2}\mathrm{d}\tau\dot{x}_c^2 \tag{B.134}$$

In that limit, the action S_c is simply the instanton action S_I. Using the definition of $\psi_1^{(0)}$, we have

$$\int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \left[\psi_1^{(0)}(\tau)\right]^2 = \frac{1}{m\left[\dot{x}_c(-\beta/2)\right]^2} \cdot S_I \tag{B.135}$$

In the next paragraphs, we will show that

$$\psi_2^{(0)}(\beta/2) = m\left[\dot{x}_c(-\beta/2)\right]^2 \frac{\partial \beta}{\partial E}, \tag{B.136}$$

which directly gives us

$$\boxed{\frac{\partial}{\partial \theta} \frac{\det_a(\mathcal{O}+\theta)}{\det_a(\mathcal{O}_{\mathrm{HO}})}\bigg|_{\theta=0} = e^{-\omega\beta} \frac{\partial \beta}{\partial E} S_I} \tag{B.137}$$

Computing $\psi_2^{(0)}(\beta/2)$:

The first thing to notice is that we have been lying to you and hiding problems under the rug. The definition of $\psi_2^{(0)}(\tau)$ from eq. (B.120),

$$\psi_2^{(0)}(\tau) = \psi_1^{(0)}(\tau) \int_{-\beta/2}^{\tau} \frac{\mathrm{d}\tau'}{\left[\psi_1^{(0)}(\tau')\right]^2}, \tag{B.138}$$

is only valid for negative τ. Indeed, $\psi_1^{(0)}(\tau)$ vanishes at $\tau = 0$, which is the turning point of the associated classical trajectory. At $\tau \to 0_-$, we are "saved" since the prefactor goes to 0 while the integral diverges. However, at $\tau > 0$, $\psi_2^{(0)}$ is simply not well defined.

There is a trick to express $\psi_2^{(0)}(\beta/2)$ in a different way. Define a even function $\psi_{\mathrm{even}}(\tau)$ such that

$$\psi_2^{(0)}(\tau) = \psi_{\mathrm{even}}(\tau) + C\psi_1^{(0)}(\tau) \tag{B.139}$$

This has the following nice properties:

- Evaluating the above equation (B.139) at $\tau = \pm\beta/2$, we find

  $$\psi_2^{(0)}(\beta/2) = -2C. \tag{B.140}$$

  Therefore, if we find C, we have solved our problem.

- Using boundary properties of $\psi_{1,2}^{(0)}(\tau)$, one can show that

  $$\dot{\psi}_{\mathrm{even}}(-\beta/2) = 1 \tag{B.141}$$

  Furthermore, since ψ_{even} is even, its derivative is odd and therefore

  $$\dot{\psi}_{\mathrm{even}}(0) = 0. \tag{B.142}$$

- Taking the derivative of (B.139), we find

$$\dot{\psi}_2^{(0)}(\tau) = \dot{\psi}_{\text{even}}(\tau) + C\dot{\psi}_1^{(0)}(\tau) \tag{B.143}$$

and by definition (B.120),

$$\dot{\psi}_2^{(0)}(\tau) = \dot{\psi}_1^{(0)}(\tau) \int_{-\beta/2}^{\tau} \frac{\mathrm{d}\tau'}{[\psi_1^{(0)}(\tau')]^2} + \frac{1}{\psi_1^{(0)}(\tau)} \tag{B.144}$$

We can then compute:

$$C = \int_{-\beta/2}^{\tau} \frac{\mathrm{d}\tau'}{[\psi_1^{(0)}(\tau')]^2} + \frac{1}{\psi_1^{(0)}(\tau)\dot{\psi}_1^{(0)}(\tau)} - \frac{\dot{\psi}_{\text{even}}(\tau)}{\dot{\psi}_1^{(0)}(\tau)} \tag{B.145}$$

This is valid at any $\tau < 0$, and in particular we can take the limit $\tau \to 0_-$. The last term above vanishes since $\dot{\psi}_{\text{even}}$ is odd and is therefore 0 at $\tau = 0$, and $\dot{\psi}_1^{(0)}(0) \neq 0$. We therefore have

$$C = \lim_{\tau \to 0_-} \left[\int_{-\beta/2}^{\tau} \frac{\mathrm{d}\tau'}{[\psi_1^{(0)}(\tau')]^2} + \frac{1}{\psi_1^{(0)}(\tau)\dot{\psi}_1^{(0)}(\tau)} \right] \tag{B.146}$$

Both terms diverge in the limit $\tau \to 0_-$, but their sum is finite. Using the definition of $\psi_1^{(0)}(\tau)$ in terms of $x_c(\tau)$, we have

$$C = [\dot{x}_c(-\beta/2)]^2 \lim_{\tau \to 0_-} \left[\int_{-\beta/2}^{\tau} \frac{\mathrm{d}\tau'}{[\dot{x}_c(\tau')]^2} + \frac{1}{\dot{x}_c(\tau)\ddot{x}_c(\tau)} \right] \tag{B.147}$$

Using the properties of x_c, we find

$$C = [\dot{x}_c(-\beta/2)]^2 \lim_{\tau \to 0_-} \left[\int_0^{x_c(\tau)} \frac{\mathrm{d}x}{\left[\frac{2(E+V(x))}{m}\right]^{3/2}} + \frac{1}{\dot{x}_c(\tau)\ddot{x}_c(\tau)} \right] \tag{B.148}$$

Finally, we can relate this to β by noticing that

$$\beta = 2\int_{-\beta/2}^{0} \mathrm{d}\tau = \lim_{y \to 0_-} 2\int_0^{x(E)+y} \frac{\mathrm{d}x}{\dot{x}_c} \tag{B.149}$$

$$\tag{B.150}$$

where $x(E)$ is the turning point, and we introduced the limit $y \to 0_-$ since the integrand diverges at $x_c = x(E)$. The turning point verifies

$$V(x(E)) = -E \implies V'(x(E))\frac{\partial x(E)}{\partial E} = -1, \tag{B.151}$$

and by taking the τ derivative of the equation of motion, we find

$$V'(x_c(\tau)) = m\ddot{x}_c(\tau) \tag{B.152}$$

Evaluating at $\tau \to 0_-$, we finally have

$$\frac{\partial x(E)}{\partial E} = -\frac{1}{m\ddot{x}_c(0)} \tag{B.153}$$

Taking the derivative of β with respect to E, we find

$$\frac{\partial \beta}{\partial E} = 2 \lim_{y\to 0_-} \frac{\partial}{\partial E} \int_0^{x(E)+y} \frac{\mathrm{d}x}{\sqrt{\frac{2(E+V(x))}{m}}} \tag{B.154}$$

$$= 2 \lim_{y\to 0_-} \left[\frac{\partial x(E)}{\partial E} \frac{1}{\sqrt{\frac{2(E+V(x(E)+y))}{m}}} - \frac{1}{m} \int_0^{x(E)+y} \frac{\mathrm{d}x}{\left[\frac{2(E+V(x))}{m}\right]^{3/2}} \right] \tag{B.155}$$

$$= -\frac{2}{m} \lim_{\tau\to 0_-} \left[\frac{1}{\ddot{x}_c(\tau)\dot{x}_c(\tau)} + \int_0^{x_c(\tau)} \frac{\mathrm{d}x}{\left[\frac{2(E+V(x))}{m}\right]^{3/2}} \right] \tag{B.156}$$

$$\tag{B.157}$$

where we identified

$$x_c(\tau) = x(E) + y \tag{B.158}$$

in the limits $\tau \to 0_-$ and $y \to 0_-$. This then tells us that

$$\psi_2^{(0)}(\beta/2) = -2C = m[\dot{x}_c(-\beta/2)]^2 \frac{\partial \beta}{\partial E} \tag{B.159}$$

as promised in equation (B.136)! We therefore indeed have equation (B.137):

$$\boxed{\frac{\partial}{\partial \theta} \frac{\det_a(\mathcal{O}+\theta)}{\det_a(\mathcal{O}_{\mathrm{HO}})}\bigg|_{\theta=0} = e^{-\omega\beta} \frac{\partial \beta}{\partial E} S_I} \tag{B.160}$$

We now have an expression for the energy splitting (see all the way back to equation B.98):

$$\boxed{E_1 - E_0 = 2\hbar e^{-\frac{1}{\hbar}S_I} \sqrt{\frac{S_I}{2\pi\hbar}} \left(e^{-\omega\beta} \frac{\partial \beta}{\partial E} S_I \right)^{-1/2}}, \tag{B.161}$$

where we are as usual working in the large β limit, and therefore the $E \to 0_-$ limit. Therefore, we can write the energy splitting as

$$E_1 - E_0 = 2\hbar e^{-\frac{1}{\hbar}S_I} \left(-\frac{2\pi\hbar}{\omega} \frac{\partial}{\partial E} e^{-\omega\beta(E)} \right)^{-1/2} \tag{B.162}$$

Finally, we can simplify this expression in the specific case of our potential by computing $\beta(E)$ in the $E \to 0_-$ limit. Here is what will happen: in the limit $E \to 0_-$, β diverges and therefore $e^{-\omega\beta}$ goes to 0. However, if β diverges **logarithmically** with E, we would have $e^{-\omega\beta(E)} \sim E \cdot (\text{finite piece})$. In that case, taking the derivative would get rid of the factor of E and we would get a nice closed form expression for the energy splitting. In the next paragraph we present the asymptotic behavior of $\beta(E)$ as $E \to 0_-$.

Computing $\beta(E)$ in the $E \to 0_-$ limit:
We have

$$\beta(E) = 2\int_0^{x(E)} \mathrm{d}x \sqrt{\frac{m}{2(E+V(x))}} \tag{B.163}$$

In the limit $E \to 0_-$, $x(E) \to a$ and the integral diverges since $V(a) = 0$. We would like to understand how exactly this integral diverges. To do so, we isolate the divergence by adding and subtracting the harmonic approximation of the potential near a (shown in green in figure B.4).

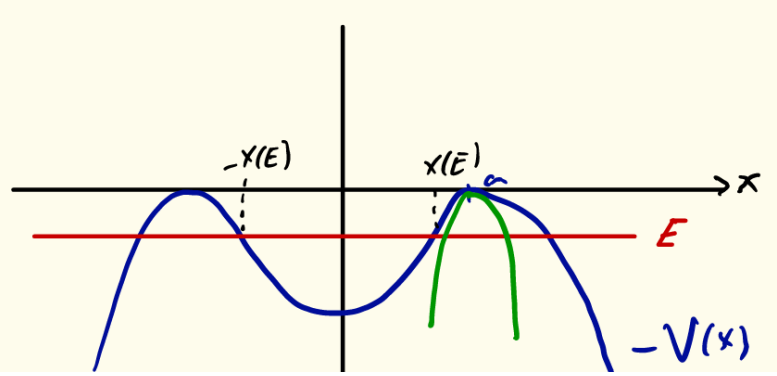


Figure B.4: Inverted potential $-V(x)$. Near $x = a$, the potential is approximated by the quadratic function $-\frac{1}{2}m\omega^2(x-a)^2$, shown in green.

In equations, we have

$$\beta(E) = \sqrt{2m}\int_0^{x(E)} \mathrm{d}x \left[\frac{1}{\sqrt{E+V(x)}} - \frac{1}{\sqrt{E+\frac{1}{2}m\omega^2(x-a)^2}} + \frac{1}{\sqrt{E+\frac{1}{2}m\omega^2(x-a)^2}}\right] \tag{B.164}$$

$$= \sqrt{2m}\int_0^{x(E)} \mathrm{d}x \left[\frac{1}{\sqrt{E+V(x)}} - \frac{1}{\sqrt{E+\frac{1}{2}m\omega^2(x-a)^2}}\right] + \sqrt{2m}\int_0^{x(E)} \mathrm{d}x \left[\frac{1}{\sqrt{E+\frac{1}{2}m\omega^2(x-a)^2}}\right] \tag{B.165}$$

Now the first term above is no longer divergent at $E \to 0_-$, since we subtracted a term

that behaves exactly like $\frac{1}{\sqrt{V(x)}}$ near $x = a$. Therefore, it can be written as

$$I_1 \equiv \sqrt{2m} \int_0^{x(E)} \mathrm{d}x \left[\frac{1}{\sqrt{E + V(x)}} - \frac{1}{\sqrt{E + \frac{1}{2}m\omega^2(x-a)^2}} \right] \tag{B.166}$$

$$= \int_0^a \mathrm{d}x \left[\sqrt{\frac{2m}{V(x)}} - \frac{2}{\omega(a-x)} \right] + \mathcal{O}(E) \tag{B.167}$$

$$= \underbrace{-\frac{2}{\omega} \int_0^a \mathrm{d}x \left[-\sqrt{\frac{m\omega^2}{2V(x)}} + \frac{1}{a-x} \right]}_{\text{finite}} + \mathcal{O}(E) \tag{B.168}$$

The divergence is therefore contained in the second term of (B.165). We can use the relation

$$E = -V(x(E)) = -\frac{1}{2}m\omega^2(x(E)-a)^2 + \mathcal{O}((x(E)-a)^3) \tag{B.169}$$

From this we deduce that E and $(x(E)-a)^2$ have the same behaviour as $E \to 0$, which implies $\mathcal{O}((x(E)-a)^3) = \mathcal{O}(E^{3/2})$, and therefore

$$I_2 \equiv \sqrt{2m} \int_0^{x(E)} \mathrm{d}x \left[\frac{1}{\sqrt{E + \frac{1}{2}m\omega^2(x-a)^2}} \right] \tag{B.170}$$

$$= \frac{2}{\omega} \int_0^{x(E)} \mathrm{d}x \left[\frac{1}{\sqrt{(x-a)^2 - (x(E)-a)^2 + \mathcal{O}(E^{3/2})}} \right] \tag{B.171}$$

Exercise B.2 (Computing the integral)**.**
Show that

$$\int_0^{x(E)} \frac{dx}{\sqrt{(x-a)^2 - (x(E)-a)^2 + \mathcal{O}(E^{3/2})}} = \ln\left(\frac{2a}{a - x(E)}\right) + \mathcal{O}(E^{1/4}) \tag{B.172}$$

Therefore, we have

$$I_2 \xrightarrow{E \to 0_-} \frac{1}{\omega} \ln\left(\frac{2m\omega^2 a^2}{-E}\right) \tag{B.173}$$

and we find

$$\beta(E) \xrightarrow{E \to 0_-} \frac{1}{\omega} \ln\left(\frac{2m\omega^2 a^2}{-E}\right) - \frac{2}{\omega} \int_0^a \mathrm{d}x \left[\frac{1}{a-x} - \sqrt{\frac{m\omega^2}{2V(x)}} \right]. \tag{B.174}$$

Hence,

$$\frac{\partial}{\partial E} e^{-\omega\beta(E)} \xrightarrow{E\to 0_-} \frac{-1}{2m\omega^2 a^2} \exp\left(2\int_0^a \mathrm{d}x \left[\frac{1}{a-x} - \sqrt{\frac{m\omega^2}{2V(x)}}\right]\right) \tag{B.175}$$

which finally implies

$$\boxed{E_1 - E_0 = 2\hbar\omega e^{-\frac{1}{\hbar}S_I} \left(\frac{m\omega a^2}{\pi\hbar}\right)^{1/2} \exp\left(-\int_0^a \mathrm{d}x \left[\frac{1}{a-x} - \sqrt{\frac{m\omega^2}{2V(x)}}\right]\right)} \tag{B.176}$$

Application to the double well potential
For the case $V(x) = \frac{\lambda}{4!}(x^2 - a^2)^2$, with $\frac{\lambda a^2}{3} = m\omega^2$, the integral in the exponential reads

$$I \equiv \int_0^a \mathrm{d}x \left[\frac{1}{a-x} - \sqrt{\frac{m\omega^2}{2V(x)}}\right] \tag{B.177}$$

$$= \int_0^a \mathrm{d}x \left[\frac{1}{a-x} - \frac{2a}{a^2-x^2}\right] = -\ln(2) \tag{B.178}$$

which implies

$$\boxed{E_1 - E_0 = 4\hbar\omega\sqrt{\frac{3}{\pi\bar{\lambda}}} e^{-\frac{2}{\bar{\lambda}}}}, \tag{B.179}$$

where $\bar{\lambda}$ is the dimensionless coupling defined in (3.135).

Appendix C

Exercises

Quantum Physics IV, Exercises 1

Exercise 1 (Gaussian integral)**:**
For all integrals below: $\alpha > 0$.

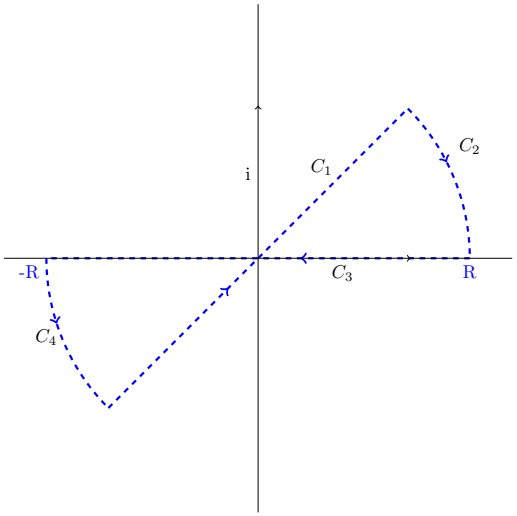
- Compute the value of the real Gaussian integral[1]

$$G_{\text{Re}} = \int_{-\infty}^{+\infty} \mathrm{d}x \; e^{-\alpha x^2}$$

- Now we will compute the Gaussian integral

$$G_{\text{Im}}^{\pm} = \int_{-\infty}^{+\infty} \mathrm{d}x \; e^{\pm i\alpha x^2} \tag{C.1.1}$$

  - By considering the complex version of the function above and by applying Cauchy's Theorem we can relate the previous two integrals. Consider the integral over the closed contour shown below[2]. Take the limit $R \to \infty$,



  - Find appropriate parametrizations for the curves $C_{1,2,3,4}$.
  - Show that the integrals over C_2 and C_4 vanish for $R \to \infty$.[3]
  - Use these results to compute $G_{\text{Im}}^{\pm}$.

- Compute, for all $n \in \mathbf{N}^+$, $\alpha > 0$[4]

$$\int_{-\infty}^{\infty} x^n e^{-\alpha x^2} \tag{C.1.2}$$

[1] Hint: Take the square and change to polar coordinates.
[2] Hint: For the exponent with $-\alpha$ you should take a different contour. Which one?
[3] Hint: Show that the absolute value vanishes. Use Euler's formula.
[4] Hint: You can exchange integration and derivation when integrating a continuous function with a continuous first derivative.

- Estimate the error when approximating the two integrals below by sending $L \to \infty$:

$$G^L_{\text{Re}} = \int_{-L}^{+L} \mathrm{d}x\ e^{-\alpha x^2} \quad \text{and} \quad G^L_{\text{Im}} = \int_{-L}^{+L} \mathrm{d}x\ e^{+i\alpha x^2}$$

  - Rewrite the first integral as $\int g(x) \frac{d}{dx} e^{-x^2}$ and apply partial integration to show that you get an order $e^{-\alpha L^2}/L$ term.
  - Show that the other term(s) are of higher order in $1/L$ (this can be done by repeatedly applying the method of the previous step and finding a smaller and smaller extra term).
  - How does this change if we take the imaginary integral? What does this mean for its rate of convergence.

Exercise 2 (Multi-dimensional Gaussian integral)**:**
A is a n-dimensional symmetric positive definite matrix. Compute the n dimensional real Gaussian integral: [5]

$$G_A(0) = \int_{-\infty}^{+\infty} \mathrm{d}^n x\ e^{-\sum_{i,j} A_{ij} x_i x_j}$$

and the imaginary Gaussian integral:

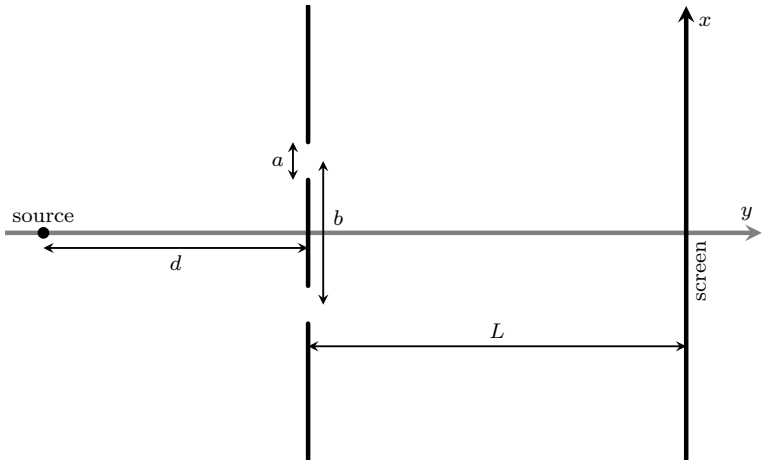
$$G_A(0) = \int_{-\infty}^{+\infty} \mathrm{d}^n x\ e^{i\sum_{i,j} A_{ij} x_i x_j} \tag{C.1.3}$$

What changes?

Now generalize this for when there is an linear "current" term (repeated indices are summed over). [6]

$$G_A(J) = \int_{-\infty}^{+\infty} \mathrm{d}^n x\ e^{-iA_{ij} x_i x_j + iJ_i x_i} \tag{C.1.4}$$

Exercise 3 (Double slit experiment)**:**



[5] Hint: You will need to diagonalize A.
[6] Hint: Complete the square so that you can apply the previous result.

In this exercise you are going to be guided through a quantitative discussion of the double slit experiment. The main goal of the exercise is to determine for which ranges of values of the parameters of the experiment (size of the slits, distance to the screen, etc.) will you be able to successfully observe the interference pattern of the electron wavefunctions. Assume the electrons are emitted from a thermionic lamp with a temperature T, and answer the following questions:

1. For a physical lamp, the electrons can be treated non-relativistically. Why is that? And what does that mean quantitatively?[7]

2. What are the two conditions that the length scales in the problem need to satisfy for the wavefunctions to be well approximated by spherical waves after passing through the slits?

3. Assume $L \gg b$. Show that, in this regime, the wavefunction evaluated on the screen is
$$|\psi_{\text{tot}}(x,t)|^2 \propto \cos^2(\alpha x)\,, \tag{C.1.5}$$
using that
$$\psi_i(x,t) = \frac{A_i}{|\mathbf{x}-\mathbf{x}_i|} e^{i\left(\frac{p|\mathbf{x}-\mathbf{x}_i|}{\hbar} - \frac{Et}{\hbar} + \phi_i\right)} \tag{C.1.6}$$
are the components of the wavefunction represented as spherical waves centered in $\mathbf{x}_i$, the position of the two slits. The electron momentum is p, E is the energy and ϕ_i the phase of each component wavefunction. The origin $\mathbf{x} = 0$ is taken to be the middle point of the screen. Compute α and derive the position of the first maximum.

4. Let's say we want the position of the first maximum to be more than $x = 2mm$ away from the main maximum, such that we can observe it. For which values of L, in terms of the other scales in the problem, is this condition satisfied?

Exercise 4 (Splitting an exponential of non-commuting operators)**:**
The exponent of a sum of non-commuting operators is not simply the product of the exponents of the individual operators. (How can you instantly see that this cannot be correct?). Instead we can split the exponent using the Zasserhaus formula[8]
$$e^{t(X+Y)} = e^{tX}\; e^{tY}\; e^{-\frac{t^2}{2}[X,Y]}\; e^{\frac{t^3}{6}(2[Y,[X,Y]]+[X,[X,Y]])} \dots \tag{C.1.7}$$
Use this to show that
$$\langle p|e^{\epsilon\left(\hat{T}+\hat{V}\right)}|x\rangle = e^{\epsilon(T(p)-iV(x))}\,\langle p|e^{-\epsilon^2 C}|x\rangle = e^{\epsilon(T(p)-iV(x))}\,\langle p|x\rangle + \mathcal{O}(\epsilon^2)\,, \tag{C.1.8}$$
assuming $\hat{T} = T(\hat{p}) = \frac{-i\hat{p}^2}{2m}$, and that $\hat{V} = -iV(\hat{x})$ is a function $\hat{x}$ only.

[7] Hint: Use Boltzmann's constant $k_B = 0.86 \times 10^{-4}$ eV/K and the electron energy at rest $m_e c^2 = 0.511 MeV$.

[8] This formula is often referred to as the Baker-Campbell-Hausdorff formula, from which it is actually derived.

In the lecture we will encounter this term when we consider the transition amplitude for going from x to x'

$$\langle x'|e^{-iH\epsilon}|x\rangle = \int dp \, \langle x'|p\rangle \, \langle p|e^{-iH\epsilon}|x\rangle \tag{C.1.9}$$

Neglecting the higher order epsilon corrections we can rewrite this integral into the following form

$$\int \frac{dp}{2\pi\hbar} \exp\left[-i\epsilon\left(\frac{p^2}{2m} + V(x) - \frac{m\dot{x}^2}{2}\right)\right] \tag{C.1.10}$$

At which order in ϵ the corrections neglected in (C.1.8) will contribute to the integral (C.1.9)? [9]

[9] Hint: Notice that $p \propto \epsilon^{-1/2}$.

Quantum Physics IV, Exercises 2

Exercise 5 (Free particle propagator)**:**
In this exercise, you will compute the free particle ($\mathcal{L} = m\dot{x}^2/2$) propagator using the path integral approach.

a) As a first step, compute the free particle propagator using basic quantum mechanics methods: starting from the definition

$$K(x_f, t; x_i, 0) = \langle x_f | \, e^{-\frac{i}{\hbar}Ht} \, |x_i\rangle \ , \tag{C.2.1}$$

insert the identity in momentum space, and compute the resulting gaussian integral to show that

$$K(x_f, t_f, x_i, t_i) = \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} \exp\left[\frac{im}{2\hbar(t_f - t_i)}(x_f - x_i)^2\right] \tag{C.2.2}$$

b) Now, we can look at the problem from the path integral point of view. As you saw in the lecture, the propagator can be expressed as

$$K(x_f, t_f, x_i, t_i) = \lim_{\epsilon\to 0} \frac{1}{A} \int \prod_{k=1}^{N-1} \frac{dx_k}{A} e^{\frac{i}{\hbar}S} \, , \tag{C.2.3}$$

where $A = \sqrt{\frac{2\pi i\epsilon\hbar}{m}}$ and where the time interval was split into steps of size $\epsilon = \frac{t_f - t_i}{N}$ (this is the same as what was done in the lecture).

Take $x_0 \equiv x_i$ and $x_N \equiv x_f$. Show that $S = \sum_{k=0}^{N-1} \frac{m}{2} \frac{(x_{k+1} - x_k)^2}{\epsilon}$ and perform the x_1 integral[10]. To recognize the pattern of these integrals you may also want to do the x_2 integral. Then show that the n-th integral will give

$$\int dx_n \exp\left[\frac{im}{2\epsilon\hbar}\left(\frac{1}{n}(x_n - x_0)^2 + (x_{n+1} - x_n)^2\right)\right] = \sqrt{\frac{2\pi i\epsilon\hbar}{m}\frac{n}{n+1}} \exp\left[\frac{im}{2\epsilon\hbar}\left(\frac{1}{n+1}(x_{n+1} - x_0)^2\right)\right] \tag{C.2.4}$$

Using all these results, check that your result for the propagator matches with part A).

[10]Hint: there are two terms in which x_1 occurs. One involving x_0 and one involving x_2. After integrating out x_1 you find an exponent involving the difference between x_2 and x_0.

Exercise 6 (Schrodinger equation)**:**
Given a wave function $\psi(x_0, t_0)$ at a time t_0, the following equation gives the wave function at a time t:

$$\psi(x,t) = \int_{-\infty}^{+\infty} \mathrm{d}x_0 K(x,t;x_0,t_0)\psi(x_0,t_0) \tag{C.2.5}$$

1. Show this by using $K(x,t,x_0,t_0) = \langle x|\, e^{-iH(t-t_0)}\, |x_0\rangle$.

In the rest of this exercise, you will show that this equation holds the same information as the Schrodinger equation. To see that, consider the evolution over an infinitesimal time interval ϵ. By matching the small ϵ expansion of the left hand side and the right hand side of (C.2.5), you will rediscover Schrodinger's equation.

2. Take t to be $t_0 + \epsilon$. For small ϵ we can approximate the integral over all paths in K by the contribution of a small straight path over a single time step of size ϵ. Compute the action

$$S = \int_{t_0}^{t_0+\epsilon} \mathrm{d}t \Big(\frac{1}{2} m\dot{x}^2 - V(x) \Big) \tag{C.2.6}$$

for a straight path with boundary conditions $x(t_0) = x_0$ and $x(t_0+\epsilon) = x$. With this action in hand, convince yourself that the propagator should take the form:

$$K(x, t_0+\epsilon, x_0, t_0) \approx \frac{1}{\mathcal{N}} e^{\frac{i}{\hbar}\left[\frac{m}{2}\frac{(x-x_0)^2}{\epsilon} - \epsilon V\left(\frac{x+x_0}{2}\right)\right]}, \tag{C.2.7}$$

where we keep $\mathcal{N}$ as a variable to be determined.

3. Show that, after making a change of variables, equation (C.2.5) leads to

$$\psi(x, t_0+\epsilon) \approx \frac{1}{\mathcal{N}} \int_{-\infty}^{+\infty} \mathrm{d}\delta\, e^{\frac{i}{\hbar}\left[\frac{m}{2}\frac{\delta^2}{2\epsilon} - \epsilon V\left(x+\frac{\delta}{2}\right)\right]} \psi(x+\delta, t_0). \tag{C.2.8}$$

4. Argue that we can expand around $\delta = 0$ and do so. To what order should you expand? Pay attention to the relation between orders of ϵ and orders of δ. This relation can best be seen after integrating the Gaussian integral(s) over δ.

5. Matching the order ϵ^0 terms on both sides, find $\mathcal{N}$

6. Matching the order ϵ terms on both sides, rediscover the Schrodinger Equation.

Exercise 7 (A Primer in Variational Calculus)**:**
Functional integrals are maps from the space of functions to the set of real (or complex) numbers. Functional derivatives are defined as follows

$$\frac{\delta F}{\delta f(x_0)} = \lim_{\epsilon\to 0} \frac{F[f(x) + \epsilon\delta(x-x_0)] - F[f(x)]}{\epsilon}, \tag{C.2.9}$$

where x is the variable of integration. Use this definition to compute the functional derivatives of the following functional integrals

$$\begin{aligned} F_1[f] &= \int f(x)\mathrm{d}x\,, \qquad F_2[f] = \int (f(x))^p \phi(x)\mathrm{d}x\,, \\ F_3[f] &= \int g[f(x)]\mathrm{d}x\,, \qquad F_4[x] = \int \left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 \mathrm{d}t\,, \\ F_5[f] &= \int G(x,y) f(x)\mathrm{d}x\,, \qquad F_6[J] = e^{-\frac{1}{2}\int \mathrm{d}x\mathrm{d}y J(x)\Delta(x-y)J(y)}\,. \end{aligned} \tag{C.2.10}$$

Use these tools to determine whether the classical trajectories of the free particle and of the harmonic oscillator are minimal, maxima or saddle points of the action. To do so, you need to examine the second order functional derivative of the action $\delta^2 S[x,\dot{x}]$.[11]

[11] Hint: You will need to integrate by parts $\delta\dot{x}$, and then appropriately expand δx in eigenfunctions of the differential operator you will obtain.

Quantum Physics IV, Exercises 3

Exercise 8 (Free particle propagator)**:**
Remember the following identities/definitions:

$$K(x_f, t_f; x_i, t_i) = \int_{x(t_i)=x_i,\, x(t_f)=x_f} \mathcal{D}[x] \exp\left(\frac{i}{\hbar} S\right), \tag{C.3.1}$$

$$\mathcal{D}[x] = \frac{1}{A} \prod_{i=1}^{N-1} \frac{dx_i}{A}, \qquad A = e^{-i\pi/4} \sqrt{\frac{m}{2\pi\hbar\epsilon}}, \qquad \epsilon = \frac{t_f - t_i}{N}. \tag{C.3.2}$$

a) We will once more compute the propagator $K(x_f, t_f; x_i, t_i)$ for a free particle. But this time we will use determinant methods.

- Start by showing that

$$K(x_f, t_f; x_i, t_i) = \exp\left[\frac{im}{2\hbar} \frac{(x_f - x_i)^2}{t_f - t_i}\right] K(0, t_f; 0, t_i). \tag{C.3.3}$$

  Hint: write $S[x(t)]$ as $S[x_{cl}(t) + y(t)]$ with x_{cl} the solution to the equations of motion so that you can express the exponent in K as $S[x_{cl}] + S[y]$ with $y(t_i) = y(t_f) = 0$.

- Next we need to compute $K(0, t_f, 0, t_i)$. We could do this explicitly by discretizing time, but in this exercise you will use a different and arguably faster method: using Gelfand-Yaglom's theorem.

  As you have seen during lecture 3, Gelfand-Yaglom's theorem is a formula to compute the propagator for a harmonic oscillator with time-dependent frequency[12].

  The theorem tells us that

$$K(0, t_f, 0, t_i) = \sqrt{\frac{m}{2\pi i\hbar\varphi(t_f)}} \tag{C.3.4}$$

  where φ is the solution to $\ddot{\varphi}(t) + \omega^2(t)\varphi(t) = 0$, such that $\varphi(t_i) = 0$ and $\dot{\varphi}(t_i) = 1$ ($\omega^2(t)$ is the time-dependent frequency of the harmonic oscillator).

  Use this to compute $K(0, t_f, 0, t_i)$ in the case of free particle.

[12] More generally, any quadratic action can be cast into a form suitable for the use of Gelfand-Yaglom's theorem

b) Using the free particle propagator determine the evolution of a gaussian wave-packet

$$\psi(x, t = 0) = \mathcal{N} \exp\left(-x^2/2\sigma_0^2\right) \exp(-ipx/\hbar) \tag{C.3.5}$$

What happens to the mean and the variance of the probability density $|\psi(x,t)|^2$?

c) We want to interpret $K(x, t; 0, 0)$ as a wave function $\psi(x, t)$. This will help us develop an better intuition about this object.

- What is the corresponding wave-function at time $t = 0$? Can you guess the probability density in the momentum space?
- Determine the associated probability density both in coordinate and in momentum space?

Exercise 9 (Some analytical mechanics and path integral identities)**:**
Prove the following statements :

a)

$$\mathrm{d}_{t_f} S_{\mathrm{cl}} = -E \quad \text{and} \quad \mathrm{d}_{x_f} S_{\mathrm{cl}} = P, \tag{C.3.6}$$

where S_{cl} is the action evaluated on the classical trajectory and fixed end-point variations are assumed.

Hint: write $x_{cl}(t) = f(x_f, t_f, x_i, t_i, t)$: the classical path $x_{cl}(t)$ depends implicitly on x_f, x_i, t_f, t_i, and the function f makes that dependence explicit. Then,

$$f(x_f, t_f, x_i, t_i, t = t_i) = x_i \tag{C.3.7}$$
$$f(x_f, t_f, x_i, t_i, t = t_f) = x_f \tag{C.3.8}$$

The trick is then to take *total* derivatives of the above relations with respect to x_i, t_i, x_f, t_f. As a reminder, recall that for a function $g(x, y)$, we have

$$\frac{\mathrm{d}}{\mathrm{d}x} g(x, y = x) = \Big[\frac{\partial g}{\partial x} + \frac{\partial g}{\partial y} \underbrace{\frac{\partial y}{\partial x}}_{=1}\Big]_{y=x} \tag{C.3.9}$$

b)

$$\int \mathcal{D}[x(t)] \left(\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}\dot{x}}\right) e^{\frac{i}{\hbar}S[x]} = 0 \tag{C.3.10}$$

Hint: consider a small, *fixed* deviation $\delta(t)$ which vanishes at the boundary. Then, do a change of variables in the path integral: $x(t) = y(t) + \delta(t)$. What happens to the measure $\mathcal{D}[x(t)]$? You should be able to conclude after computing the quantity $S[y + \delta]$ to leading order.

Exercise 10 (Saddle point approximation)**:**
Consider the integral :

$$I(\alpha) = \int_C e^{\alpha f(z)} g(z) \mathrm{d}z \tag{C.3.11}$$

where α is real, f and g are analytic in some region of the complex plane containing the contour C. We would like to compute an approximation to this integral when α is large. Often such integrals can be approximated using the saddle point (or steepest descent) method:[13]

$$I(\alpha) \approx g(z_0)e^{\alpha f(z_0)}\sqrt{\frac{2\pi}{\alpha}}\frac{e^{i\theta_1}}{\sqrt{|f''(z_0)|}} \tag{C.3.12}$$

where z_0 satisfies $f'(z_0) = 0$ and θ_1 is the angle of the path passing through z_0, chosen such that $0 \leq \theta_1 < \pi$, $2\theta_1 + \theta_2 = \pi$ or 3π, where θ_2 is the phase of $f''(z_0)$.

1. Apply this approximation to two examples :

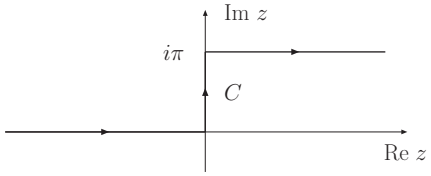
   - Stirling formula for large N:

   $$N! = \Gamma(N+1) = \int_0^\infty \mathrm{d}x\ e^{-x}x^N$$

   - Hankel function for large α:

   $$H_\nu^{(1)}(\alpha) = \frac{1}{i\pi}\int_C \frac{e^{\alpha\frac{1}{2}(z-1/z)}}{z^{\nu+1}}\mathrm{d}z$$

   where the contour C is :



You are now going to be guided through the general proof of this approximation.

2. To start, argue that the integral

   $$I(\alpha) = \int_C e^{\alpha f(z)}g(z)\mathrm{d}z \tag{C.3.13}$$

   is dominated by the contribution coming from the point z_0 in the path such that $\mathrm{Re}f(z_0)$ is a maximum. Argue that we need to choose a contour along which $\mathrm{Im}f(z)$ is constant close to z_0. [14]

3. Argue that a point of the contour that maximizes $\mathrm{Re}f(z)$ and has $\mathrm{Im}f(z)$ constant is a saddle point of $f(z)$ (by this we mean a saddle point of both $\mathrm{Re}f(z)$ and of $\mathrm{Im}f(z)$). That is why this is called the saddle point approximation.

[13] A condition for these methods to work is that $f(z)$ has a saddle point. Further comments on the conditions at the end of this exercise.

[14] Remember that two contours are equivalent if you can deform one into the other without crossing any singularity. That means that in the quest to approximate $I(\alpha)$ we are free of choosing the contour that optimizes our approximation.

4. Taylor expand $f(z)$ to second order around this saddle point z_0. Call $z - z_0 \equiv r_1 e^{i\theta_1}$ and $\frac{1}{2}f''(z_0) \equiv r_2 e^{i\theta_2}$. Show that, close to z_0, the path along which $\mathrm{Im}[f(z)] - \mathrm{Im}[f(z_0)]$ is constant is also the path along which $\mathrm{Re}[f(z)] - \mathrm{Re}[f(z_0)]$ is maximized. That is the path we want. By requiring the constancy of $\mathrm{Im} f(z)$ we have fixed θ_1 in terms of θ_2, which by definition is the phase of $f''(z_0)$. That is why this method is also called "of steepest descent".

5. Having made this choice, we now have

$$f(z) - f(z_0) = -r_1^2 r_2 \equiv -t^2 = \frac{1}{2}(z - z_0)^2 f''(z_0)\,. \tag{C.3.14}$$

Taylor expand $g(z)$ around z_0 and perform a change of variable from z to t. You then should obtain the so-called asymptotic expansion of $I(\alpha)$:

$$I(\alpha) \approx e^{\alpha f(z_0)} \sum_{k=0}^{\infty} \frac{2^{k+\frac{1}{2}} e^{i(2k+1)\theta_1}}{|f''(z_0)|^{k+\frac{1}{2}}(2k)!} g^{(2k)}(z_0) \Gamma\left(k + \frac{1}{2}\right) \alpha^{-k-\frac{1}{2}}\,. \tag{C.3.15}$$

Check that the first term in this expansion is exactly the saddle point approximation (C.3.12) . We have used that

$$\int_{-\infty}^{\infty} e^{-\alpha t^2} t^n \mathrm{d}t = \alpha^{-\frac{n+1}{2}} \Gamma\left(\frac{n+1}{2}\right)\,. \tag{C.3.16}$$

Here are some extra comments on the saddle point approximation and its applicability:

- To properly understand the large α behaviour of the integral (C.3.11) one should start by doing a contour plot of $\mathrm{Re}\, f(z)$ for $z \in \mathbb{C}$. Then one can deform the integration contour towards the minimal values of $\mathrm{Re}\, f(z)$ until the contour is always orthogonal to the lines of constant $\mathrm{Re}\, f(z)$. [15]

- Sometimes it can happen that the maximum of $\mathrm{Re} f(z)$ is not at a saddle point of $f(z)$, but at the end-points of the contour. In addition, it is possible that while deforming towards the optimal contour one encounters a singularity of g. In this case, the integral may be dominated by this singularity. Often the function $\mathrm{Re}\, f(z)$ has several saddle points and drawing the optimal contour is important to identify what is the relevant saddle point.

[15] One may think of $\mathrm{Re}\, f(z)$ as a height function over $\mathbb{C} = \mathbb{R}^2$. Then let the original contour "fall" like a tensionless string in this landscape keeping the endpoints fixed. The final contour will be steepest descent in the landscape.

Quantum Physics IV, Exercises 4

Exercise 11 (Propagator for the harmonic oscillator)**:**
The propagator for the harmonic oscillator has the following form

$$K_{HO}(x_f, T; x_i, 0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}} \exp\left[\frac{i}{\hbar} S_{cl}\right] \tag{C.4.1}$$

where S_{cl} is the action evaluated on the solutions of the equations of motion obtained with Dirichlet boundary conditions $x_{cl}(0) = x_i$, $x_{cl}(T) = x_f$.

a) Use Gelfand-Yaglom's theorem to recover the prefactor

$$K_{HO}(0, T; 0, 0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}} \tag{C.4.2}$$

b) Calculate the explicit expression for $K_{HO}(x_f, T; x_i, 0)$.

c) Consider a gaussian wave packet at rest at time $t = 0$

$$\psi(x, 0) = \frac{1}{(2\pi\sigma_0^2)^{\frac{1}{4}}} e^{-\frac{(x-x_0)^2}{4\sigma_0^2}}, \tag{C.4.3}$$

where the prefactor is such that

$$\int_{-\infty}^{\infty} |\psi(x, 0)|^2 \mathrm{d}x = 1\,. \tag{C.4.4}$$

Determine the wave function at later time $t = T$, if the dynamics are those of a harmonic oscillator. [16]

d) Read off the averages $\overline{x}(t) = \langle x(t)\rangle$, and $\Delta x(t)^2 = \langle (x(t) - \overline{x}(t))^2\rangle$ and discuss their relation w.r.t. the classical problem.

Hint: Recall that for a gaussian wave-packet $\psi(x) = N \exp\left(-\frac{(x-x_0)^2}{4\sigma_0^2}\right)$, $\overline{x} = x_0$ *and* $\Delta x^2 = \sigma_0^2$.

Exercise 12 (More Propagators)**:**
For both systems below compute the propagator. The idea is to make use of the known solutions (free particle and harmonic oscillator) :

$$\begin{aligned} K_{\text{free}}(x, t; 0, 0) &= \sqrt{\frac{m}{2\pi i\hbar t}} e^{\frac{i}{\hbar} S_{\text{cl}}^{\text{free}}} \\ K_{\text{HO}}(x, t; 0, 0) &= \sqrt{\frac{m\omega}{2\pi i\hbar |\sin(\omega t)|}} e^{i(n_+ - n_-)\frac{\pi}{4}}\ e^{\frac{i}{\hbar} S_{\text{cl}}^{\text{HO}}} \end{aligned}$$

[16] Hint: The calculations here become cumbersome. Remember that Mathematica is your friend.

1. Constant gravitational field :

$$\mathcal{L}_{\text{grav.}} = \tfrac{1}{2}m\dot{x}^2 - mgx$$

2. Forced harmonic oscillator :

$$\mathcal{L}_{\text{forced HO}} = \tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}m\omega^2 x^2 - J(t)x$$

To solve the forced harmonic oscillator, here is some guidance:

- To start, write x as the classical solution x_{cl} to the **unforced** harmonic oscillator plus a path y. You should get:

$$S_{\text{forced HO}}[x] = S_{\text{forced HO}}[x_{cl}] - \frac{1}{2}\int_0^T dt\big[y\ \underbrace{m\left(\frac{d^2}{dt^2}+\omega^2\right)}_{D_\omega} y + 2J(t)y\big]$$

- At the end of the first exercise session we saw that

$$x^T Ax + J^T x = (x + JA^{-1}/2)^T A(x + A^{-1}J/2) - J^T A^{-1}J/4 \equiv x'^T Ax' - J^T A^{-1}J/4. \tag{C.4.5}$$

We will now use the continuous equivalent of this. We need to find the 'inverse' of the differential operator D_ω. To this end we assume that there is a function $G(t,\tau)$ such that

$$D_\omega G(t,\tau) = \delta(t-\tau) \quad , \quad G(0,\tau) = G(T,\tau) = 0 \tag{C.4.6}$$

We will find this G explicitly later. We introduce the notation

$$G \cdot J \equiv \int dt'\, G(t,t')J(t'). \tag{C.4.7}$$

Rewrite the y dependent part of the action as:

$$S_y = -\frac{1}{2}\int dt\,(y(t) + G\cdot J(t))D_\omega(t)(y(t) + G\cdot J(t)) + \frac{1}{2}\int dt\,dt'\,J(t')G(t',t)J(t). \tag{C.4.8}$$

- You should shift the integration path again such that you obtain

$$K_{\text{forced HO}}(x_f, T, x_i, 0) = e^{\frac{i}{\hbar}S_{\text{forced HO}}[x_{cl}] + \frac{i}{2\hbar}J\cdot G\cdot J}\int_{y(0)=0}^{y(T)=0} D[\bar{y}]e^{\frac{i}{\hbar}S_{\text{HO}}[\bar{y}]}\,. \tag{C.4.9}$$

What was the shift $y \to \bar{y}$? Why will the boundary conditions on our new $\bar{y}$ be the same as the ones on y?

- Now we only need to evaluate the factors in front of the path integral. In order to do this, we will have to find the explicit expression for $G(t,\tau)$. We will need to solve the differential equation (C.4.6). First write the general solution for $t < \tau$ and $t > \tau$. Note that in these domains we have a simpler homogeneous differential equation $D_\omega G = 0$. You should find:

$$G_\pm(t,\tau) = R_\pm(\tau)\sin(\omega t + \phi_\pm) \tag{C.4.10}$$

where $\pm$ stands for $t < \tau$, $t > \tau$.

- Use the continuity of G and the discontinuity of the first derivative of G ,

$$G_-(\tau,\tau) = G_+(\tau,\tau) \tag{C.4.11}$$

$$G'_+(\tau,\tau) - G'_-(\tau,\tau) = \frac{1}{m}, \tag{C.4.12}$$

  as well as the boundary conditions, to find $\phi_\pm$ and $R_\pm$. Can you derive (C.4.12) ?
- Use all these elements to compute the full propagator.

Quantum Physics IV, Exercises 5

Exercise 13 (Wick rotations and 2-point functions)**:**
In the lecture, you defined the Euclidean vacuum expectation value

$$G_E(\tau_1, \tau_2) \equiv \langle 0| T\hat{x}_E(\tau_1)\hat{x}_E(\tau_2) |0\rangle , \tag{C.5.1}$$

where $\hat{x}_E(\tau) = e^{\frac{1}{\hbar}H\tau}\hat{x}_E e^{-\frac{1}{\hbar}H\tau}$ is the Heisenberg picture Euclidean position operator[17] and T is the time-ordering operator which places the $\hat{x}_E$ with highest τ on the left, and the others in decreasing order to the right.

The Minkowski space correlator can be obtained by **Wick rotation** $\tau \to it$ in the above:

$$\langle 0| T\hat{x}(t_1)\hat{x}(t_2) |0\rangle = G_E(it_1, it_2) \tag{C.5.2}$$

In this exercise, you will familiarize yourself with the Wick rotation by looking in greater details at the 2pt function without the time-ordering.

- Show that $\langle 0| \hat{x}_E(\tau_1)\hat{x}_E(\tau_2) |0\rangle$ is well-defined only if

  $$\mathrm{Re}(\tau_1) > \mathrm{Re}(\tau_2) \tag{C.5.3}$$

  Hint: use the fact that the Hamiltonian is in general not bounded from above.

- Wick-rotating consists of setting $\tau_j = e^{i\alpha}t_j$ $(j = 1, 2)$ and going from $\alpha = 0$ (Euclidean) to $\alpha = \frac{\pi}{2}$ (Minkowski). Draw the τ complex plane to visualize the rotation. Is the constraint (C.5.3) realized during the whole rotation? Which 2pt function do you obtain?

- Assume now that we want to compute the **unordered** Minkowski 2pt function[18]

  $$\langle 0| \hat{x}(t_1)\hat{x}(t_2) |0\rangle , \quad t_1 < t_2 \tag{C.5.4}$$

  Is it possible to reach this from the Euclidean correlator using the same rotation as before?

- Instead of rotating τ_1 and τ_2 in the same way with a parameter α as above, consider now the case $\tau_j = it_j + \epsilon_j$ $(j = 1, 2)$, where $\epsilon_j \ll 1$. Is it possible to pick ϵ_1 and ϵ_2 such that

  $$\langle 0| \hat{x}(t_1)\hat{x}(t_2) |0\rangle \tag{C.5.5}$$

  is well defined? Again, draw the τ complex plane to better visualize what you are doing.

[17] Note that it is obtained by replacing $t \to -i\tau$ in the usual Minkowski space operator $\hat{x}(t)$.
[18] In QFT, these are sometimes called Wightman functions

- Convince yourself that in Minkowski space, it is possible to define out of time order correlators starting from time-ordered Euclidean correlators by using the above prescription. Try to generalize the discussion to 3-point functions and above. Can you find an explicit parametrization of the ϵ?

Exercise 14 (The propagator of the forced harmonic oscillator in Euclidean time)**:**
We will now find the propagator for the HO with source in Euclidean time

$$K_E^{\text{fHO}}(x_i, x_f; \beta) = \int_{\substack{x(0)=x_i \\ x(\beta)=x_f}} \mathcal{D}[x] \, \exp\left(-\frac{S_E^J}{\hbar}\right) \tag{C.5.6}$$

with

$$S_E^J[x] = \int_0^\beta d\tau \left(\frac{m}{2}\dot{x}^2 + \frac{m\omega^2}{2}x^2 + J(\tau)x\right) \tag{C.5.7}$$

We now have to do a computation that is similar to what we did last week. However, here we have rotated to euclidean time $\tau = it$.

- Start from the definition of the Minkowski propagator of the forced harmonic oscillator from last week exercise sheet and perform a Wick rotation to check that you obtain (C.5.6). In particular, check that this changes the exponent to be of the form $-\frac{S_E^J}{\hbar}$ and check that the signs in the (now Euclidean) action S_E (C.5.7).

- Now, we can proceed similarly as last week in order to find the explicit form of the Euclidean propagator. (You may want to go back to last week exercise sheet for guidance.). After performing the usual change of variable $x = x_{cl} + y$ where x_{cl} is the classical solution of the unforced HO, you should obtain

$$K_E^{\text{fHO}}(x_i, x_f; \beta) = \exp\left(-\frac{S_E^J[x_{cl}] + \frac{1}{2}J \cdot G_E \cdot J}{\hbar}\right) K_E^{HO}(0, 0; \beta) \tag{C.5.8}$$

  where

$$D_\omega^E G_E(\tau_1, \tau_2) = \delta(\tau_1, \tau_2), \quad G_E(0, \tau) = G_E(\beta, \tau) = 0 \tag{C.5.9}$$

  with $D_\omega^E = m\left(\frac{d^2}{dt^2} - \omega^2\right)$ (notice the sign change compare to the Minkiwski case).

- Following the same steps as last week, we can now find the different terms of (C.5.8) and obtain

$$K_E^{\text{fHO}}(x_i, x_f; \beta) = \sqrt{\frac{\omega}{2\pi\hbar\sinh(\omega\beta)}} \exp\left[-\frac{\frac{1}{2}m\omega\frac{(x_f^2+x_i^2)\cosh(\omega\beta)-2x_i x_f}{\sinh(\omega\beta)} + J \cdot x_{cl} + \frac{1}{2}J \cdot G_E \cdot J}{\hbar}\right]$$

Exercise 15 (Partition function of HO)**:**
We want to compute the thermal partition function of the HO given by

$$Z(\beta) = \int \mathrm{d}X \; K_E^{\text{HO}}(X, X; \beta) \; . \tag{C.5.10}$$

a) Use the result of Ex.2 to compute explicitly the partition function, you should obtain

$$\boxed{Z(\beta) = \frac{1}{2\sinh(\omega\beta/2)}} \tag{C.5.11}$$

b) Rewrite the partition function in order to obtain the energy levels of the harmonic oscillator. You will need the series expansion for $1/(1-x)$. Then, compare with

$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta E_n/\hbar} \tag{C.5.12}$$

Exercise 16 (Van Vleck-Pauli-Morette formula)**:**
We saw that for a generic quadratic hamiltonian the propagator can be found using the Gelfand-Yaglom theorem:

$$K(0, t_f, 0, t_i) = \sqrt{\frac{m}{2\pi i\hbar\phi(t_f)}} \tag{C.5.13}$$

Moreover, even when dealing with a potential of higher order we can do a semi-classical approximation where we expand the action to second order in the variation y around the classical path x_{cl}. For an action of the form

$$S[x] = \int \left(\frac{m\dot{x}^2}{2} - V(x)\right) dt \tag{C.5.14}$$

This gives

$$K(x_f, t_f, x_i, t_i) \approx K^{\text{semi-classical}}(x_f, t_f, x_i, t_i) = e^{\frac{iS[x_{cl}]}{\hbar}} \int \mathcal{D}[y] e^{\frac{i}{\hbar}\int \mathrm{d}t\left[\frac{m\dot{y}^2}{2} - \frac{1}{2}\frac{\delta^2 V}{\delta x^2}(x_{\mathrm{cl}})y^2\right]}, \tag{C.5.15}$$

where we used that linear terms in y have a vanishing contribution. Then, we can apply Gelfand Yaglom's theorem with $\Omega(t) = V''(x_{cl}(t))$. We just need to find $\phi(t_f)$, the solution to

$$\left(\frac{d^2}{dt^2} + \frac{\Omega(t)}{m}\right)\phi(t) = 0 \tag{C.5.16}$$

satisfying the boundary conditions $\phi(t_i) = 0$ and $\dot{\phi}(t_i) = 1$.

a) To start, differentiate the classical equations of motion to show that $\dot{x}_{\mathrm{cl}}$ is a solution of (C.5.16).

b) Unfortunately, $\dot{x}_{\mathrm{cl}}$ does not satisfy the right boundary conditions. To find the solution that does, we are going to use the Wronskian. In general, if you have found $n-1$ solutions to a order n differential equation, the Wronskian will help you finding the last solution. Given two functions f and g, their Wronskian is defined as

$$W(t) = f(t)\dot{g}(t) - \dot{f}(t)g(t)\,. \tag{C.5.17}$$

Given the one solution we found, $v(t) \equiv \dot{x}_{cl}(t)$, we write the Wronskian with the solution we seek, $\phi(t)$, as

$$W(t) = v(t)\dot{\phi}(t) - \dot{v}(t)\phi(t)\,, \tag{C.5.18}$$

Using (C.5.16), show that

$$\dot{W}(t) = 0. \tag{C.5.19}$$

c) Show that $\dot{W}(t) = 0$ implies

$$\frac{d}{dt}\left(\frac{\phi(t)}{v(t)}\right) = \frac{v(t_i)}{v^2(t)} \tag{C.5.20}$$

d) Solve this differential equation to find $\phi(t_f)$. With a simple change of variable you should find that the solution can be expressed as an integral over x:

$$\phi(t_f) = v(t_f)v(t_i)\int_{x_i}^{x_f} \frac{\mathrm{d}x}{v(x)^3} \tag{C.5.21}$$

e) Finally, we want to write our result in terms of the action. To do so, show that[19]

$$\frac{\partial^2 S_{\mathrm{cl}}}{\partial x_i \partial x_f} = \frac{1}{v(t_f)}\frac{\partial E}{\partial x_i}\,, \tag{C.5.22}$$

and

$$\frac{\partial E}{\partial x_i} = -\frac{m}{v(t_i)\int_{x_i}^{x_f}\frac{\mathrm{d}x}{v^3(x)}}\,. \tag{C.5.23}$$

You should obtain, in the end,

$$K^{\text{semi-classical}}(x_f, t_f, x_i, t_i) = e^{\frac{iS[x_{cl}]}{\hbar}}\sqrt{-\frac{1}{2\pi i\hbar}\frac{\partial^2 S_{cl}}{\partial x_i \partial x_f}}\,. \tag{C.5.24}$$

This is called the Van Vleck-Pauli-Morette formula for semiclassical propagators.

[19] What you showed in Exercise Sheet 3 will come useful here.

Quantum Physics IV, Exercises 6

Exercise 17 (Partition function of the forced HO)**:**
Compute the partition function of the forced HO or equivalently the partition function of the HO coupled to an external source.[20]

$$Z_{\mathrm{HO}}[\beta, J] = \int_{x\left(-\frac{\beta}{2}\right)=x\left(\frac{\beta}{2}\right)} \mathcal{D}[x] \exp\left[-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} d\tau \mathcal{L}^E_{\mathrm{HO}} - J(\tau)x(\tau)\right] \tag{C.6.1}$$

where

$$\mathcal{L}^E_{\mathrm{HO}} = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2 x^2 \tag{C.6.2}$$

- Completing the square, you should obtain

$$Z_{\mathrm{HO}}[\beta, J] = Z_{\mathrm{HO}}(\beta, 0) \exp\left[\frac{J \cdot G_P \cdot J}{2\hbar}\right] \tag{C.6.3}$$

  where the Green's function is the solution of

$$\underbrace{m\left(-\partial_{\tau_1} + \omega^2\right)}_{D_\omega} G_P(\tau_1, \tau_2) = \delta(\tau_1 - \tau_2) \tag{C.6.4}$$

  with periodic boundary condition (why?)

$$G_P\left(-\frac{\beta}{2}, \tau_2\right) = G_P\left(\frac{\beta}{2}, \tau_2\right) \tag{C.6.5}$$

$$\partial_{\tau_1} G_P\left(-\frac{\beta}{2}, \tau_2\right) = \partial_{\tau_1} G_P\left(\frac{\beta}{2}, \tau_2\right) \tag{C.6.6}$$

- Use the continuity equation at $\tau_1 = \tau_2$ and the periodic boundary condition to show that

$$G_P(\tau_1, \tau_2) = \frac{1}{2\omega m} \frac{\cosh\left[\omega\left(\frac{1}{2}\beta - |\tau_1 - \tau_2|\right)\right]}{\sinh\left(\frac{1}{2}\omega\beta\right)} \tag{C.6.7}$$

- Conclude by using last week's result for the unforced HO:

$$Z_{\mathrm{HO}}(\beta, 0) = \frac{1}{2\sinh\left(\omega\beta/2\right)} \ . \tag{C.6.8}$$

Exercise 18 (Perturbative expansion & anharmonic oscillator)**:**
Consider a harmonic oscillator perturbed by an anharmonic term :

$$\mathcal{L}_E = \tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}m\omega^2 x^2 + \frac{\lambda}{4!}x^4$$

We will treat the quartic interaction as a small perturbation, that is $\lambda \ll 1$ and will study the partition function. The aim is to compute :

[20] Note that we defined here $J(\tau)$ with opposite sign compared to last week. The reason is that we want to match the equation studied in the lectures

- Mean energy at first order in λ.
- Free energy to second order in λ in small and large β limit.

Definitions :

$$\text{Free energy :} \quad F(\beta) = -\hbar \frac{1}{\beta} \log Z$$
$$\text{Mean energy :} \quad E(\beta) = -\hbar \frac{\mathrm{d}}{\mathrm{d}\beta} \log Z$$

You will need the result derived in exercise 1.

Let us also clarify notations, we define

$$Z[\beta, J] = \int_{x\left(-\frac{\beta}{2}\right)=x\left(\frac{\beta}{2}\right)} \mathcal{D}[x] \exp\left[-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} d\tau \mathcal{L}_E - J(\tau)x(\tau)\right] \tag{C.6.9}$$

and

$$Z[\beta] \equiv Z[\beta, 0] = \int_{x\left(-\frac{\beta}{2}\right)=x\left(\frac{\beta}{2}\right)} \mathcal{D}[x] \exp\left[-\frac{1}{\hbar}\int_{-\beta/2}^{\beta/2} d\tau \mathcal{L}_E\right] \tag{C.6.10}$$

---

1. First we need to find an expression for the perturbed partition function in terms of functional derivatives acting on the unperturbed partition function that we know. Starting from

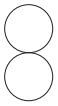
$$Z[\beta] = \int_{x\left(-\frac{\beta}{2}\right)=x\left(\frac{\beta}{2}\right)} D[x] \exp[-(S_{\mathrm{HO}} + S_{\mathrm{int.}})/\hbar], \tag{C.6.11}$$

show that

$$Z[\beta] = Z_0[\beta] \exp\left[-\frac{\lambda}{\hbar 4!}\int \mathrm{d}\tau_1 \left(\frac{\hbar\delta}{\delta J(\tau_1)}\right)^4\right] \exp\left(\frac{1}{2\hbar} J \cdot \mathtt{G} \cdot J\right)\Big|_{J=0}. \tag{C.6.12}$$

What are $Z_0[\beta]$ and $\mathtt{G}(\tau_1, \tau_2)$?

2. Now we can find $Z[\beta]$ to any order in λ by expanding the exponent to the appropriate order. We see that the functional derivative to $J(\tau_n)$ can act in different ways to give different contributions (either working on one of the J's in the exponent or on J's that were brought down by previous functional derivatives). Start by explicitly calculating the first order partition function (in terms of G). Check that you understand that we can represent the result by (a numerical factor times) the following diagram:

 . (C.6.13)

You can see that there is a diagrammatic way to work out what contractions of G you can get by acting with a functional derivative with respect to J and how often

such a contraction occurs. For instance for the diagram we just saw we knew we had access to one vertex (one order of λ). All functional derivatives were at the same point (the same τ coordinates). Thus, all four lines need to connected back to the same vertex. So the only option is to connect them all back. However, we are left with the choice of how to do this. Take one line, we have to connect this line to one of three others. This gives 3 options. This was the only choice as the two lines that are left have to connect to each other. This choice corresponds to the fact that we can get $G(\tau_1, \tau_1)^2$ in three different ways by acting with functional derivatives. Thus, we can work out the combinatorics of the derivatives using only the diagrams.

3. Now calculate the second order contribution both explicitly and diagrammatically and check that the results match. You will now find disconnected diagrams. In fact you will find the previous diagram twice. (Take a look at the numerical pre-factor. Are you starting to see a pattern?) Calculate the pre-factor of the diagram consisting of three such disconnected diagrams (which you find at the third order calculation) and see whether you understand the pattern.

4. Show that we can write these disconnected diagrams as the exponential of the connected one, show especially that the pre-factors work out. In general all disconnected diagrams can be written as the exponential of connected ones. When you take the log of the partition function (free energy) you will get only connected diagrams.

5. Write the partition function at order 0, 1 and 2 in terms of diagrams (pay attention to the multiplicities), and write $\log[Z(\beta)]$ also in terms of diagrams.

6. Compute the first order diagram exactly (do the integral over the greens function),

7. Compute the second order ones in the small β limit. (It is a good exercise to also calculate the large β limit now. However, it might actually be easier to obtain it later when we have the exact expression.)

8. We will need an integral identity for the next level. So here is a small mathematical interlude. Show the following identity:

$$\int \cosh^n(x)\mathrm{d}x = \frac{n-1}{n}\int \cosh^{n-2}(x)\mathrm{d}x + \frac{1}{n}\cosh^{n-1}(x)\sinh(x)$$

and use it to obtain :

$$\int \cosh^2(x)\mathrm{d}x = \tfrac{1}{2}x + \tfrac{1}{4}\sinh(2x)$$
$$\int \cosh^4(x)\mathrm{d}x = \tfrac{3}{8}x + \tfrac{1}{4}\sinh(2x) + \tfrac{1}{32}\sinh(4x)$$

9. Use the integrals above to compute the second order diagrams exactly. Check the limits obtained earlier.

10. Compute the mean energy at first order. Identify a dimensionless expansion parameter.

11. Compute the free energy at second order in the small and large β limits. Identify the dimensionless expansion parameter for each limit.

12. Discuss the validity of the expansion, give an interpretation of the conclusion in both limits and relate the two expansion parameters.

Quantum Physics IV, Exercises 7

Exercise 19 (Free energy of HO perturbed by a cubic potential)**:**
Consider a harmonic oscillator perturbed by a cubic term :

$$\mathcal{L}_E = \tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}m\omega^2 x^2 + \frac{\lambda}{3!}x^3$$

and compute the leading correction to the ground state energy. Here is some guidance:

a) Write down the partition function in terms of a path integral, and write the interaction in terms of functional derivatives acting on a source.

b) Use the periodic Greens function and the unperturbed harmonic oscillator partition function as calculated before[21]

$$\begin{aligned} G_P(\tau_1,\tau_2) &= \frac{1}{2\omega m}\frac{\cosh\left[\omega\left(\frac{1}{2}\beta - |\tau_1-\tau_2|\right)\right]}{\sinh\left(\frac{1}{2}\omega\beta\right)}\,, \\ Z_0[\beta] &= \frac{1}{2\sinh(\omega\beta/2)}\,, \end{aligned} \tag{C.7.1}$$

and compute the leading order correction to the partition function using Feyman diagrams. You should find that the first non-zero contribution is at $O(\lambda^2)$. Was there a way to see this from the beginning?

c) Use this result to derive the leading order correction to the free energy. What limit do you need to take in order to derive the correction to the ground state energy starting from the correction to the free energy?

Exercise 20 (1 & 2 point correlators for cubic and quartic perturbations)**:**
Compute :

a) the first non vanishing correction (*leading order* (LO) correction) to the thermal correlation functions $\langle\hat{x}\rangle$ and $\langle\hat{x}^2\rangle$ both for a harmonic oscillator perturbed by a cubic and a quartic term. Note that this is not necessarily the first order in λ. It should be easy to predict when these will vanish. Also take the large β limits.

b) the second non vanishing correction (*next to leading order* (NLO) correction) to $\langle\hat{x}\rangle$ for the cubic potential (For simplicity, in this second point, just write the diagrams, do the combinatorics and check the cancellation of the disconnected graphs. Leave evaluating the integrals for last.).

Remember :

$$\begin{aligned} \langle\hat{x}^n\rangle &= \hbar^{n/2}G_P(\tau_1=\tau,\ldots,\tau_n=\tau) \\ \hbar^{n/2}G_P(\tau_1,\ldots,\tau_n) &= \frac{1}{Z[\beta,0]}\frac{\hbar\delta}{\delta J(\tau_1)}\cdots\frac{\hbar\delta}{\delta J(\tau_n)}Z[\beta,J]\Big|_{J=0} \end{aligned}$$

[21] Or quickly re-derive the partition function from its trace definition. Since you know E_n.

Useful relations :

$$\begin{aligned}
\int \mathrm{d}x \sinh^n(x) &= \frac{1}{n} \sinh^{n-1}(x) \cosh(x) - \frac{n-1}{n} \int \mathrm{d}x \sinh^{n-2}(x) \\
\int \mathrm{d}x \cosh^n(x) &= \frac{1}{n} \cosh^{n-1}(x) \sinh(x) + \frac{n-1}{n} \int \mathrm{d}x \cosh^{n-2}(x)
\end{aligned}$$

Quantum Physics IV, Exercises 8

Exercise 21 (The partition function in the high temperature limit.)**:**
The goal of this exercise is to find the leading quantum corrections to the euclidean partition function in the $\beta \to 0$ limit. Consider the euclidean action

$$S_E = \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \left[\frac{m}{2} \dot{x}^2 + V(x) \right]. \tag{C.8.1}$$

The partition function can be written as

$$\int_{-\infty}^{\infty} dX \int_{x(\pm\beta/2)=X} \mathcal{D}[x] e^{-\frac{S_E}{\hbar}} = \int_{x(-\beta/2)=x(\beta/2)} \mathcal{D}[x] e^{-\frac{S_E}{\hbar}}. \tag{C.8.2}$$

First way

a) Approximate the left hand side of eq. (C.8.2) by evaluating the potential on the fixed path $x(\tau) = X$ (in the $\beta \to 0$ limit, it is a reasonable first approximation to treat $V(x)$ as a constant on the interval). Can you interpret the result as the partition function of a well-known system?

b) Do an expansion around the previous approximation using $x(\tau) = X + \xi(\tau)$. Keep terms up to and including second order.

   Why should this expansion be valid (i.e. why is $\xi \ll X$ in the $\beta \to 0$ limit)? (Hint: Use dimensional analysis or isolate all β dependence in a way that the β dependence of the final result is easy to understand.)

c) Simplify as much as you can (perform a shift in ξ and remember to keep track of how this affects the boundary conditions). The goal is to get a form where you can apply the previously found harmonic oscillator result

$$K(x_f, t_f; x_i, t_i) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}} \exp\left[\frac{im\omega}{2\hbar \sin \omega T} \left[\left(x_f^2 + x_i^2\right) \cos \omega T - 2x_f x_i \right] . \right]. \tag{C.8.3}$$

   Remember you should Wick rotate this to Euclidian signature by taking $T \to -i\beta$.

d) Take the limit $\beta \to 0$. If you only go to first order in the Taylor series for cosh and sinh, you will find the same result as in a), so you should take into account the second order terms.

e) Express the final result just in terms of V' (dependence on V'' can be replaced with V' dependence through partial integration)[22].

Second way (Matsubara expansion)

[22]The boundary term that you get for doing this can be discarded if $V(X) \to \infty$ as X goes to plus or minus infinity.

e) We will now compute the right hand side by expanding $x(\tau)$ in a Fourier series

$$x(\tau) = x_0 + \sum_{k\geq 1}\left[x_k^{(s)}\sin\left(\frac{2\pi k}{\beta}\tau\right) + x_k^{(c)}\cos\left(\frac{2\pi k}{\beta}\tau\right)\right]. \tag{C.8.4}$$

Verify that this expansion satisfies the correct boundary conditions.

f) Plug this expansion into the action and expand $V(x_0 + ...)$ keeping terms up to and including second order in the x_k's. Perform the Euclidean time integral. *Useful formulas:*

$$\begin{aligned}
\frac{1}{L}\int_{-L}^{L} \mathrm{d}\tau \cos\left(\frac{n\pi}{L}\tau\right)\cos\left(\frac{m\pi}{L}\tau\right) &= \delta_{nm}\\
\frac{1}{L}\int_{-L}^{L} \mathrm{d}\tau \sin\left(\frac{n\pi}{L}\tau\right)\sin\left(\frac{m\pi}{L}\tau\right) &= \delta_{nm}\\
\frac{1}{L}\int_{-L}^{L} \mathrm{d}\tau \sin\left(\frac{n\pi}{L}\tau\right)\cos\left(\frac{m\pi}{L}\tau\right) &= 0
\end{aligned}$$

g) In terms of the new variables x_0, $x_k^{(s),(c)}$ we can perform the path integral as follows

$$dX\,\mathcal{D}[x] \to \mathcal{N} dx_0 \prod_{k\geq 1} dx_k^{(s)} x_k^{(c)} \tag{C.8.5}$$

with some (infinite) normalization $\mathcal{N}$. Perform the $x_k^{(s)}$ and $x_k^{(c)}$ (Gaussian) integrals. Fix the normalization of $\mathcal{N}$ by taking $V = 0$ and comparing with the free theory results.

h) Keep only β terms up to second order and use the identity

$$\sum_{k\geq 1}\frac{1}{k^2} = \zeta(2) = \frac{\pi^2}{6} \tag{C.8.6}$$

Check that your result matches the result from the previous exercise (Use partial integration again).

Exercise 22 (The quartic integral)**:**
The goal of this exercise is to investigate some mathematical features of various kinds of approximations to the toy model of the quartic integral

$$I(g) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dz\, e^{-\frac{1}{2}z^2 - \frac{1}{4}g\,z^4}, \tag{C.8.7}$$

which is defined for $\mathrm{R}e(g) \geq 0$. This can be interpreted as the path integral of a zero dimensional anharmonic oscillator with a quartic interaction term. For interested readers, `https://munsal.files.wordpress.com/2014/10/marino-lectures2014.pdf` is a great reference.

a) Show that the series expansion around $g = 0$ is given by

$$I(g) = \sum_{n=0}^{\infty} a_n g^n \,, \qquad\qquad a_n = (-4)^{-n} \frac{(4n-1)!!}{n!} \,. \tag{C.8.8}$$

b) Show that this perturbative series is asymptotic, *i*.e. it has zero radius of convergence.

c) We would like to extend the definition of $I(g)$ to negative values of g, by keeping the integral convergent. To do so, we can analytically continue this integral by rotating g clockwise or counterclockwise by 180° and compensating by rotating z^4 by the opposite amount, such that $\mathrm{Re}(gz^4) > 0$. Show that this corresponds to rotating the contour of integration by 45° clockwise or anticlockwise.

d) Notice that these two ways of analytically continuing this integral lead to different answers. This means that $I(g)$ has a branch cut along the negative real axis. Use the saddle point approximation to compute the discontinuity along this branch cut.

e) Plot the partial sums

$$I_N(g) = \sum_{n=0}^{N} a_n g^n \,, \tag{C.8.9}$$

for $g = 0.04$ and $N = 0, 1, \ldots, 10$ and compare these values with the exact value $I(g = 0.04)$. What N should you choose to obtain the best approximation to the exact value? What happens for other values of g? Can you determine the optimal value of N as a function of g?

f) **Borel summation:** Define the Borel transform

$$F(t) = \sum_{n=0}^{\infty} \frac{1}{n!} a_n t^n \,. \tag{C.8.10}$$

Show that the function

$$\tilde{I}(g) \equiv \frac{1}{g} \int_0^{\infty} dt\, e^{-t/g} F(t) \,, \tag{C.8.11}$$

has the same perturbative expansion as $I(g)$, as long as the integral over t converges.

g) From equation (C.8.10), show that the radius of convergence of the Borel transform is finite. Evaluate (C.8.10) with Mathematica. It should give you a closed form expression. What are the singularities of $F(t)$ in the complex $t-$plane?

h) **Pade approximants:** Consider the following rational representations of the series expansion of $I(g)$:

$$P_N(g) \equiv \frac{b_0 + b_1 g + \ldots b_N g^N}{1 + c_1 g + \ldots c_N g^N} = \sum_{n=0}^{2N} a_n g^n + O(g^{2N+1}) \tag{C.8.12}$$

This is called the $[N/N]$ Pade approximant to $I(g)$. *Hint*: in order to find the b and c coefficients, impose that $\frac{\partial^n P_N(g)}{\partial g^n}\Big|_{g=0}$ matches on both sides. Do this with Mathematica for various values of N.

Check numerically that $\lim_{N\to\infty} P_N(g) = I(g)$ for any $g > 0$ (in practice, check up to $N \sim 8$). Plot the poles of $P_N(g)$ in the complex $g-$plane for several values of N.

i) Further reading at https://munsal.files.wordpress.com/2014/10/marino-lectures2014.pdf

Quantum Physics IV, Exercises 9

Exercise 23 (Free particle fixed energy propagator)**:**
The goal of this exercise is to compute the fixed energy propagator for a free particle by Fourier transforming the fixed time propagator. Start by inserting the fixed time propagator in the definition of the fixed energy propagator.[23]

$$\begin{aligned} K(T;x_f,x_i) &= \sqrt{\frac{m}{2\pi i\hbar T}}e^{iS_{\rm cl}/\hbar} \\ K(E;x_f,x_i) &= \int_0^\infty \mathrm{d}T e^{i\frac{(E+i\epsilon)}{\hbar}T}K(T;x_f,x_i) \end{aligned} \tag{C.9.1}$$

Notice that it is difficult to immediately perform the T integral. To simplify the calculation we use the momentum representation of the fixed-time propagator instead of the position one.

$$K(T;x_f,x_i) = \int_{-\infty}^{\infty}\frac{\mathrm{d}p}{2\pi\hbar}\exp\left(-i\frac{p^2T}{2m\hbar}+i\frac{p(x_f-x_i)}{\hbar}\right) \tag{C.9.2}$$

You may want to check that this is correct (by doing the Gaussian p integral). Plug this into the equation for $K(E;x_f,x_i)$ and do the T integral. Then, do the p integral, using Cauchy's theorem. You will want to rewrite the integral to the following form first:

$$-im\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{\pi}\frac{e^{i\frac{p\Delta x}{\hbar}}}{(p-p_0)(p+p_0)}$$

where $\Delta x = x_f - x_i$ and $p_0 = \sqrt{2m(E+i\epsilon)}$.

Exercise 24 (WKB Approximation Validity)**:**
Next time we will see how the path integral formalism can be used to deal with bound states and meta-stable states (tunneling). This time we will brush up on the WKB approximation using the Schrodinger equation, since it will be easier to find its region of validity:

Write the generic wave function to be solved for in the time-independent problem as

$$\psi(x) = e^{\frac{i}{\hbar}\sigma}, \qquad \sigma = \sigma_0 + \left(\frac{\hbar}{i}\right)\sigma_1 + \left(\frac{\hbar}{i}\right)^2\sigma_2 + \dots$$

and solve the Schrodinger equation perturbatively in $\hbar$.

a) First solve for σ_0 at order $\mathcal{O}(0)$ then for σ_1 at order $\mathcal{O}(\hbar)$ and finally for σ_2 at order $\mathcal{O}(\hbar^2)$.

b) Then check what $\hbar\sigma_1 \ll \sigma_0$ and $\hbar^2\sigma_2 \ll \sigma_0$ mean in terms of the physical parameters of the problem. This gives you the regimes where the WKB approximation is valid.

[23] Notice that to obtain a convergent integral we gave a small imaginary part to the energy. This is analogous to requiring that the fixed energy propagator is analytic in the upper half of the complex plane.

Exercise 25 (Large order behaviour of perturbation theory)**:**
In this exercise, we will study the correction to the ground state energy to all order in perturbation theory. In this exercise, instead of using Feynman diagrams, we will use the Schrödinger equation and a clever ansatz for the wave function[24]. Inspired from last week's exercise, what do you expect for the radius of convergence of the expansion of the ground state energy in powers of λ?

Consider the anharmonic oscillator with Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \lambda x^4 \,, \tag{C.9.3}$$

we are going to study the perturbative expansion of the ground state energy [25]

$$E_0 = \frac{1}{2} + \sum_{n=1}^{\infty} A_n \lambda^n \,. \tag{C.9.4}$$

The Schrodinger equation for this system is

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + \lambda x^4 \right] \psi(x) = E_0 \psi(x) \,. \tag{C.9.5}$$

Use the following perturbative ansatz for the ground state wave function

$$\psi(x) = \frac{1}{\pi^{1/4}} \sum_{n=0}^{\infty} \lambda^n e^{-\frac{1}{2}x^2} B_n(x) \,, \qquad B_n(x) = (-1)^n \sum_{j=1}^{2n} x^{2j} B_{n,j} \,. \tag{C.9.6}$$

a) Fix $B_0(x)$ by considering the unperturbed harmonic oscillator ($\lambda = 0$) and comparing with the usual ground state wavefunction.

b) Show that this solves the Schrodinger equation if the coefficients of these polynomials satisfy the following recursion relation:

$$2jB_{n,j} = (j+1)(2j+1)B_{n,j+1} + B_{n-1,j-2} - \sum_{p=1}^{n-1} B_{n-p,1} B_{p,j} \,, \tag{C.9.7}$$

and that $A_n = (-1)^{n+1} B_{n,1}$.

c) Implement this equation recursively on Mathematica and determine A_n for $n = 1, 2, \ldots, 50$. Compare your results with the asymptotic formula

$$A_n \approx (-1)^{n+1} 3^n \sqrt{\frac{6}{\pi^3}} \Gamma\left(n + \frac{1}{2}\right) \,, \qquad n \to \infty \,. \tag{C.9.8}$$

d) What is the radius of convergence of the series (C.9.4)?

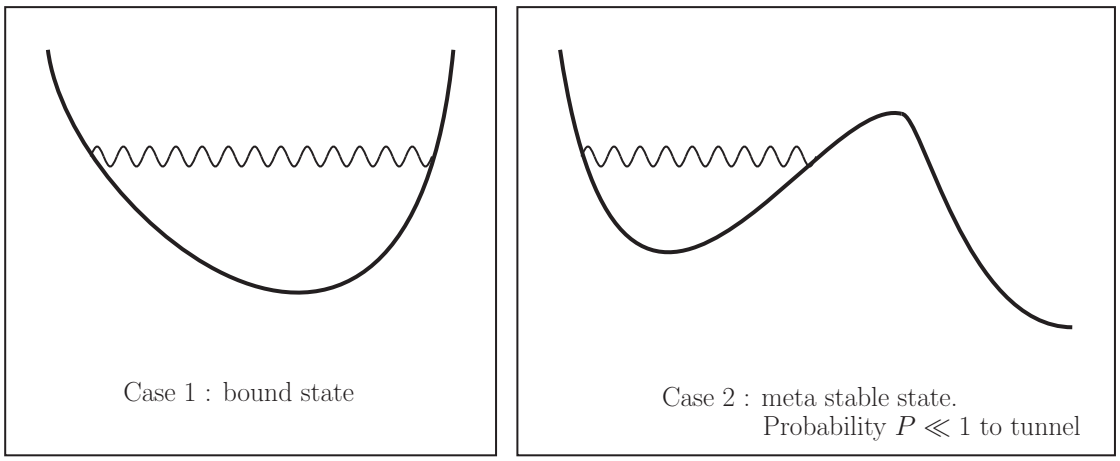
[24] The article [4] is a good reference for interested readers
[25] Notice that we are in units where $\hbar = 1$ and we choose $m = \omega = 1$ to simplify the expressions.

Quantum Physics IV, Exercises 10

Exercise 26 (Application of WKB)**:**
During the lectures, you learned about the semiclassical approximation to the fixed energy propagator

$$K_{\rm sc}(E;x_f,x_i)=\frac{1}{\sqrt{|v(x_i)v(x_f)|}}\sum_n e^{-i\frac{\pi}{2}N_n}e^{\frac{i}{\hbar}\int_{x_i}^{x_f}\mathrm{d}x_n p(x)}\,, \tag{C.10.1}$$

where $p(E,x)=\pm\sqrt{2m[E-V(x)]}$, the sum is over all classical paths of energy E, and N_n is the number of turning points of the n-th path. We will consider this approximation in the case of a bound state and of a metastable state.



Through the WKB approximation, we will compute the energy levels and the wavefunctions in both cases.
Bound state:

a) For two points x_i and x_f consider all classical paths of energy E connecting them (assume $x_f > x_i$ for simplicity). There are infinitely many. Which? Can you write the sum in equation (C.10.1) for these paths in closed form?[26]

b) Determine where the poles of the propagator are. You should find there are poles for

$$2\int_a^b p(x)\mathrm{d}x = 2\pi\hbar\big(n+\tfrac{1}{2}\big)\,. \tag{C.10.3}$$

[26]Hint: Convince yourself that all elements in the sum in equation (C.10.1) can be expressed as products of the following three factors:

$$\mathcal{D}=\exp\left(\frac{i}{\hbar}\int_{x_i}^{x_f}p(x)\mathrm{d}x\right)\,,\qquad \mathcal{L}=\exp\left(-\frac{i\pi}{2}+2\frac{i}{\hbar}\int_a^{x_i}p(x)\mathrm{d}x\right)\,,\qquad \mathcal{R}=\exp\left(-\frac{i\pi}{2}+2\frac{i}{\hbar}\int_{x_f}^{b}p(x)\mathrm{d}x\right)\,. \tag{C.10.2}$$

where a and b are the classical turning points. Then, use $\frac{1}{1-x}\approx 1+x+x^2+....$

c) To find the wavefunctions, let use an alternative form of the fixed energy propagator. Define it as the Fourier transform of the fixed time propagator in its canonical form

$$K(E; x_f, x_i) = \int_0^\infty dT \ \langle x_f | e^{-iHT/\hbar} | x_i \rangle e^{i(E+i\epsilon)T/\hbar}.$$

Carry out the time integral and write this as

$$K(E; x_f, x_i) = i\hbar \sum_n \frac{\psi_n(x_f)\psi_n^*(x_i)}{E - E_n + i\epsilon} \,. \tag{C.10.4}$$

d) Compute the residues on the poles of the expression you found in question a) and read off the wavefunctions by comparing it with Equation (C.10.4). Be careful with the denominator: when taking the residue, it will give an extra prefactor.[27]

Meta stable state:
Now there is a chance $P \ll 1$ to go over the potential barrier on each reflection. This fact can easily be incorporated in our previous calculations by changing one of the factors in Equation (C.10.2).

f) Show that the states are now unstable and decay with lifetime $\tau = \frac{T_n}{P}$.

Exercise 27 (Gravitational interference)**:**
Gravitational effects can be measured with an interferometer as shown below. A beam of neutrons, or atoms, is sent on the beam splitter in A. Half of the beam follows the path AXB, and the second half AYB. In B there is a screen which counts the number of hits. The apparatus is such that it can be rotated around the AY axis by an angle δ (see figure (C.1)).

[27] At some point you will need to show that

$$\cos\left(\frac{1}{\hbar}\int_{x_f}^{b} p(x)\mathrm{d}x - \frac{\pi}{4}\right) = (-1)^n \cos\left(\frac{1}{\hbar}\int_{a}^{x_f} p(x)\mathrm{d}x - \frac{\pi}{4}\right) . \tag{C.10.5}$$

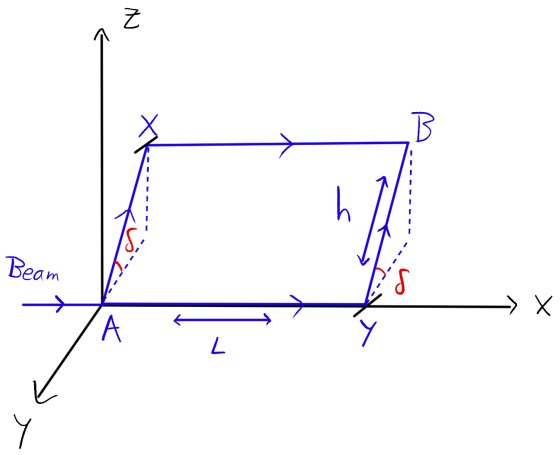


Figure C.1: A beam of particles is split at A, can be reflected at X and Y, and is detected at B. The angle δ determines the tilt of the apparatus around the AY axis.

The goal is to compute the observed interference pattern as function of δ, for a linear gravitational potential. Be careful to distinguish between the inertial mass m_i and the gravitational mass m_g[28].

a) Compute the difference between the action on the path AXB and on the path AYB. To do so, show first that one can write

$$S = \int_{path} p(x)\mathrm{d}x - E\Delta t, \quad p(x) = \sqrt{2m_i(E - V(x))} \tag{C.10.6}$$

where E is the energy of a given particle in the beam and Δt is the time it takes for the particles to go from A to B. Note that in the above, x is a schematic variable meant to indicate a spatial position, not the explicit coordinate of the x-axis.

b) Assume now that the kinetic energy of the particles is much larger than their potential energy, as is the case in these kinds of experiment. Show that

$$S_{\mathrm{AXB}} - S_{\mathrm{AYB}} = -\frac{m_i m_g L h g \sin(\delta)}{p} \tag{C.10.7}$$

c) Compute the phase shift $\Delta\phi$ between the two paths, and express the result in terms of the de Broglie wavelength $\bar{\lambda} = \frac{\hbar}{p}$.

Exercise 28 (Bloch waves and instantons)**:**
Consider a periodic potential $V(x) = V(x + a)$, with only one minimum per period. Find the description of the lowest energy band in the dilute instanton gas approximation. Assume each local minimum to be approximated by an harmonic potential with a certain ω.

[28]The inertial mass appears in the expression for the kinetic energy, while the gravitational mass appears in the gravitational potential.

To do the computation, we will use the instanton formalism to find

$$\langle n_f | \, e^{-\frac{\beta}{\hbar} H} \, | n_i \rangle \, , \tag{C.10.8}$$

where n_f and n_i label the position of two minima. Recall the different contributions from the lecture: determine the action for a given saddle point with fixed number of instantons and anti-instantons, write the overall prefactor (we can leave R as an unfixed parameter for now), sum over kink locations, and consider the multiplicity from the instanton/anti-instanton ordering.

1. Show that

$$\langle n_f | \, e^{-\beta H/\hbar} \, | n_i \rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} e^{-\beta\omega/2} \sum_{n,\bar{n}} \frac{1}{n!\bar{n}!} \left[R\beta e^{-S_0/\hbar} \right]^{n+\bar{n}} \delta_{n-\bar{n},\Delta}, \tag{C.10.9}$$

   where $\Delta = n_f - n_i$.

2. Prove that

$$\delta_{a,b} = \int_0^{2\pi} \frac{\mathrm{d}\theta}{2\pi} e^{i(a-b)\theta}, \tag{C.10.10}$$

   and use this to express equation (C.10.9) as an integral over θ. Now assume that there exists a complete set of energy eigenstates labelled by θ (we will prove this in the next bullet point). Show that

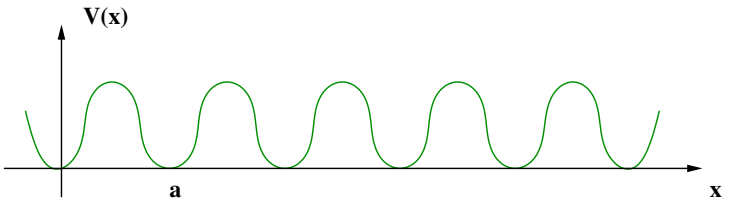
$$\langle n_f | \, e^{-\beta H/\hbar} \, | n_i \rangle = \int \mathrm{d}\theta e^{-\beta E(\theta)/\hbar} \, \langle n_f | \theta \rangle \, \langle \theta | n_i \rangle \tag{C.10.11}$$

   and use this to find the energy levels $E(\theta)$ and the Bloch wavefunctions $\langle n|\theta\rangle$.

3. Lastly, we want to show the existence of energy eigenstates $|\theta\rangle$. Consider first position eigenstates $|n\rangle$ corresponding to the bottom of each wells, i.e. $n \in \mathbb{Z}$. These are not eigenstates of the hamiltonian, but we can expand them as:

$$H \, |n\rangle = \sum_k \Delta_{n,n+k} \, |n+k\rangle \tag{C.10.12}$$

   Implicitly, this is an approximation which assumes that if we were to perform a position measurement on the state $H \, |n\rangle$, we would always find that it is in one of the wells - in other words, we neglect the probability that the position of $H \, |n\rangle$ is



outside a well.

Using this expansion, show that

$$|\theta\rangle = \sum_n e^{in\theta} |n\rangle \,, \quad \theta \in [0, 2\pi] \tag{C.10.13}$$

are eigenstates of H, which means that our derivation in 2) was correct. *Hint*: argue that $\Delta_{n,n+k}$ actually does **not** depend on n.

Exercise 29 (Hamiltonian truncation)**:**
Consider the anharmonic oscillator with Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \lambda_2 x^2 + \lambda_4 x^4 = \frac{1}{2} + a^\dagger a + \frac{\lambda_2}{2}(a^\dagger + a)^2 + \frac{\lambda_4}{4}(a^\dagger + a)^4 \,, \tag{C.10.14}$$

where we used

$$x = \frac{a + a^\dagger}{\sqrt{2}} \,, \qquad p = i\frac{a^\dagger - a}{\sqrt{2}} \,. \tag{C.10.15}$$

a) Set $\lambda_4 = 0$. The Hamiltonian is a harmonic oscillator with a re-defined frequency. Find the exact spectrum.

b) Truncate the Hilbert space to the first N eigenstates of the harmonic oscillator (with $\lambda = 0$),

$$|n\rangle \,, \qquad n = 0, 1, 2, \ldots, N-1 \,, \tag{C.10.16}$$

and build the $N \times N$ matrix $H_{nm} = \langle n| H |m\rangle$. Use a computer program to compute the lowest eigenvalues of this finite matrix for different values of λ_2, λ_4 and N. Test your program by the exact result of $\lambda_4 = 0$ that you found in first part.

c) From now on, for simplicity, take $\lambda_2 = 0$ and $\lambda_4 = \lambda$. Plot the ground state energy for $\lambda \in [0, 2]$ and $N = 1, 3, 5, 7, 9$. Add to this plot the predictions of perturbation theory in the first few orders (see exercise set 9).

d) Using your numerical results to compute the first and the second derivative of the ground state energy with respect to λ at $\lambda = 0$.

e) Compare your result with the prediction from perturbation theory. What is the minimal size of the truncation to match perturbation theory at order λ^k?

Quantum Physics IV, Exercises 11

Exercise 30 (False vacuum decay reappraisal)**:**
The goal of this exercise is to compute the rate of decay of the false vacuum for a potential of the form in figure C.2, assuming the conditions to apply the semiclassical approximation hold true. To be specific, consider, for explicit computations, the potential

$$V(x) = \frac{\lambda}{3!}(a-x)\,x^2 \equiv \frac{m\omega^2 x^2}{2} - \frac{\lambda x^3}{3!}, \qquad m\omega^2 = \frac{a\lambda}{3}. \tag{C.11.1}$$

a) Using the Schrodinger equation show that, given a wave function $\psi(t,x)$, the quantity $\rho(t,x) = |\psi(t,x)|^2$ satisfies a continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0 \tag{C.11.2}$$

for a suitable current J that you will identify. Using this observation link the decay rate (and the lifetime) of the false vacuum to the current J. Use physical intuition and dimensional analysis.

b) Let the initial wavefunction at time $t = t_i$ be the ground state of the harmonic oscillator centered in $x = 0$. This state is characterized by the wave function

$$\psi_0(y, t_i) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}y^2} \tag{C.11.3}$$

Write the wave function of the evolved state at a later time $t = t_f$ in terms of an integral in the semiclassical approximation.

c) Try to evaluate the integral you obtain using the saddle-point method. Show that no real trajectory exists that can satisfy the saddle-point constraint. You should find that the constraint is[29]

$$-ip_i - m\omega x_i = 0\,. \tag{C.11.4}$$

d) Convince yourself that, necessarily, the initial evolution of this trajectory has to be in complex time. To see that, look at

$$t = \int_{x_i}^{x_f} \frac{\mathrm{d}x}{v(x)} \tag{C.11.5}$$

and split it into the two intervals $x_i < x < a$ and $a < x < x_f$. Notice that we are working in the ground state, which in the limit $\hbar \to 0$ has energy $E \approx 0$. Call the Euclidean time interval of evolution β. Show that for $E \approx 0$, $\beta \to \infty$.

[29] Hint: to find this particular form of the constraint, use the general expression for the action

$$S = \int_{x_i}^{x_f} p\mathrm{d}x - \int_{t_i}^{t_f} E\mathrm{d}t\,.$$

e) Compute the exponential factor coming from the saddle point approximation. Notice that energy conservation imposes $E = 0$ on the whole path, simplifying the expression of the action on this trajectory.

f) Compute the prefactor coming from the saddle point approximation and thus complete the calculation of the wavefunction at time $t = t_f$. What are the decay rate and the lifetime of this metastable state, as a function of the other parameters of this system?

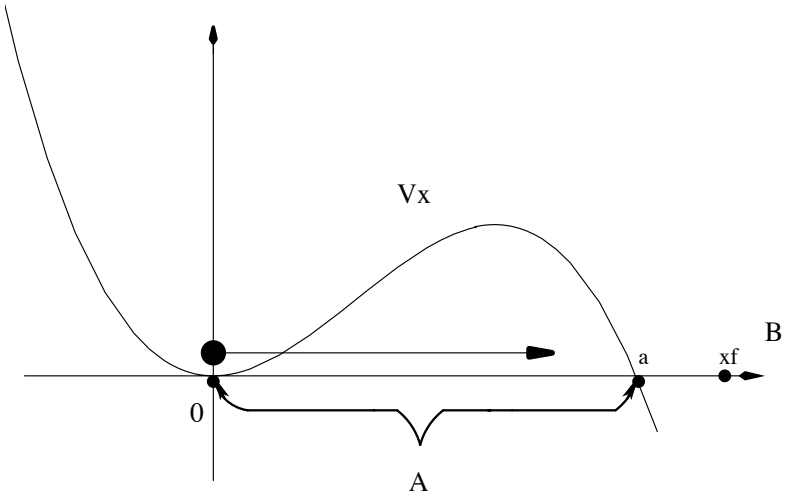


Figure C.2: Depiction of the potential $V(x)$. It has zeroes at $x = 0$ and $x = a$, and we consider $x_f > a$.

Quantum Physics IV, Exercises 12

Exercise 31 (Semiclassical evolution of a gaussian wave-packet)**:**
Consider a gaussian wave-packet at time $t = 0$

$$\psi(x) = \mathcal{N} \exp\left(-\frac{(x-\overline{x})^2}{2\Delta^2\hbar} - \frac{i}{\hbar}px\right). \tag{C.12.1}$$

We want to study its semiclassical evolution described by an action S.

a) Determine $\mathcal{N}$. Write the wave function at position $x = x_f$ at time $t = T$ in terms of an integral over the semiclassical propagator.

One expects that the wave-packet evolves in such a way that the mean remains on its classical trajectory, the gaussian shape is kept, and the width varies with time. Too see this, do a double expansion

b) Evaluate the integral over x expanding around the saddle point of the exponent. In which case does this saddle-point coincide with the center $\overline{x}$ of the initial wave-packet?.

c) Expand the wave-function at time $t = T$ around the value $x_{cl}(T)$, that is the final position of the particle moving according to its classical path.

d) Identify the width of the final wave-packet and its associated momenta.

Exercise 32 (Landau levels)**:**
Consider a particle in a constant magnetic field $\mathbf{B} = (0, 0, B)$, and choose the particular gauge $A_1 = -By$, $A_2 = A_3 = 0$ (Landau gauge).

a) Write down the Hamiltonian describing this system.

b) Check that the naive translation operator does not commute with the Hamiltonian even though the system does physically have a symmetry under translation.

c) This implies that the translations are implemented in a non-trivial way. Find the true generators of translations in presence of a magnetic field. Do they commute with the canonical momenta? Among themselves?

d) Find the energy levels and wave-functions.

Quantum Physics IV, Exercises 13

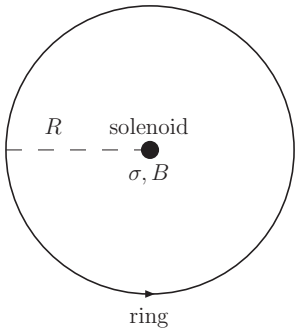
Exercise 33 (Particle on a ring)**:**
The goal of this exercise is to study how the presence of a magnetic field affects the quantum mechanical properties of a particle moving on a ring.

a) Find the energy eigenvalues and eigenfunctions of a free particle confined on a ring in the absence of a magnetic field.[30]

b) Identify the degeneracy of the free particle system. Can you relate it to the symmetries that it enjoys?

c) Now add the magnetic field. What are the new energy eigenfunctions and eigenvalues?

d) Identify the new degeneracy in the energy eigenstates (if there is any left). Can you point to some symmetry arguments to explain the reduction of degeneracy?



Exercise 34 (Magnetic monopoles and charge quantization)**:**
Maxwell's equations of electrodynamics display a strong symmetry between the electric field **E** and the magnetic field **B**. Yet magnetic charges (commonly referred to as *magnetic monopoles*) are absent: the sources of the magnetic fields we observe in nature are either moving electric charges or static magnetic dipoles, never static magnetic charges. Maxwell's equations impose $\nabla \cdot \mathbf{B} = 0$. Quantum mechanics doesn't predict nor forbid the existence of magnetic monopoles, however it clearly requires that *if magnetic monopoles exist, electric charge must be quantized and must appear in multiples of an elementary quantum of charge*. The goal of this exercise is to prove this last statement.

a) Suppose that there exists a magnetic monopole such that

$$\nabla \cdot \mathbf{B} = 4\pi\rho_M = 4\pi e_M \delta^3(x)\,. \tag{C.13.1}$$

[30] Hint: identify the correct degrees of freedom and boundary conditions.

Show that the magnetic field generated is

$$\mathbf{B} = \frac{e_M}{r^2}\hat{r}\,, \tag{C.13.2}$$

where we moved to spherical coordinates.

b) Recalling the expression of the curl in spherical coordinates[31], show that a possible choice of the vector potential that generates such a magnetic field is

$$\mathbf{A} = \frac{e_M(1-\cos\theta)}{r\sin\theta}\hat{\phi}\,. \tag{C.13.4}$$

c) Observe that the expression in (C.13.4) is not regular everywhere in space. Where is it singular?

d) Using the fact that a potential $\mathbf{A}$ regular everywhere would satisfy $\nabla\cdot(\nabla\times\mathbf{A}) = 0$, show that in the presence of a magnetic charge, such regular potential cannot exist (use Stoke's theorem).

e) Consider then two vector potentials defined in two different patches:

$$\begin{aligned} \mathbf{A}^{(1)} &= \frac{e_M(1-\cos\theta)}{r\sin\theta}\hat{\phi} \qquad \text{for} \qquad \theta \le \pi/2 \\ \mathbf{A}^{(2)} &= -\frac{e_M(1+\cos\theta)}{r\sin\theta}\hat{\phi} \qquad \text{for} \qquad \theta \ge \pi/2 \end{aligned} \tag{C.13.5}$$

On the equator $\theta = \frac{\pi}{2}$, their difference is a pure gauge: $\mathbf{A}^{(1)} - \mathbf{A}^{(2)} = \nabla\alpha$. Find α.

f) Recall the expression of the gradient in spherical coordinates:

$$\nabla\alpha = \hat{r}\frac{\partial\alpha}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial\alpha}{\partial\theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial\alpha}{\partial\phi}\,. \tag{C.13.6}$$

Consider now the wave function of an electrically charged particle of charge e and subjected to the magnetic field generated by the magnetic monopole. Since the wavefunction is not gauge invariant, its form depends on the choice of the vector potential. Find the relation between the wavefunctions $\psi^{(1)}$, $\psi^{(2)}$ corresponding to the two choices of vector potential in (C.13.5), evaluated on the equator $\theta = \frac{\pi}{2}$.

g) Using the fact that the wavefunctions must be single-valued, show that the electric charge is quantized in terms of the magnetic charge:

$$e = \frac{\hbar c}{2e_M}n\,, \qquad n = 0, \pm1, \pm2, \ldots \tag{C.13.7}$$

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[31]

$$\nabla\times\mathbf{A} = \hat{r}\left(\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(A_\phi\sin\theta) - \frac{\partial A_\theta}{\partial\phi}\right) + \hat{\theta}\frac{1}{r}\left(\frac{1}{\sin\theta}\frac{\partial A_r}{\partial\phi} - \frac{\partial}{\partial r}(rA_\phi)\right) + \hat{\phi}\frac{1}{r}\left(\frac{\partial}{\partial r}(rA_\theta) - \frac{\partial A_r}{\partial\theta}\right). \tag{C.13.3}$$

Bibliography

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