Physics Unlimited Explorer Competition

April 2022

In this competition, we will explore the path integral formulation of quantum mechanics and Feynman diagram. The path integral formulation is not what you will learn in a first course on quantum mechanics, because the Schrödinger picture turns out to be much more useful in many applications. Some of the quantities that we will calculate can be calculated more easily using Schrödinger's equation as well. However, path integral formulation is much more intuitive and conceptually simple. Path integral also has much wider applications than quantum mechanics: it turns out that most of the problems in quantum field theory can be formulated very easily using path integral, while the canonical quantization approach no longer works when you include interactions.

There are 9 sections in total and the maximum score for each exercise is put in the parenthesis. You are not expected to work out every question (we would be *very* surprised if you do manage to do that). Don't be frustrated by one or a couple questions. Most of the exercises are proof-based questions, so you can work on latter ones without relying on your previous work. There are large amounts of definitions scattered throughout this file, so if you don't know what a phrase means, you can try searching it to find its definition. Due to time limit, it is possible that this file contains typos or mistakes. If you encounter one, please let us know. This competition is designed to be self-contained, but you can use outside sources to help you understand the concepts. Good luck!

1 The Classical Action

Consider a particle moving along a straight line. The particle starts from a point x_a at an initial time t_a and goes to a final point x_b at time t_b.

The principle of least action determines the particular path $\bar{x}(t)$ out of all the possible paths *with fixed initial and final points.* The path $\bar{x}(t)$ is that for which the action S is an extremum. In classical physics, the (classical) action is defined as

$$S = \int_{t_a}^{t_b} L(x, \dot{x}, t) dt \tag{1}$$

where $L(x, \dot{x}, t) =$ Kinetic energy - Total potential energy is the Lagrangian for the system.
We can use calculus of variation to determine the extremum path $\bar{x}(t)$. Here, we will do it step by step.

1.1 Exercise: First step (1 pt)

First, let's derive formula of total differential. Consider a function with two variables $f(x_1, x_2)$. Express the change in the function upon infinitesimal changes in the two variables, $\delta x_1, \delta x_2$ and the partial differentials $\frac{\partial f}{\partial x_1}$ and $\frac{\partial f}{\partial x_2}$. (Please ignore the second order terms.)

Answer:

$$\delta f(x_1, x_2) = \frac{\partial f}{\partial x_1} \delta x_1 + \frac{\partial f}{\partial x_2} \delta x_2 \tag{S1}$$

1.2 Exercise: Second step (3 pts)

Second, the path is varied away the $\bar{x}(t)$ by a small amount $\delta x(t)$ while the end points remain fixed,i.e. $\delta x(t_a) = \delta x(t_a) = 0$. The principle of least action gives the following condition:

$$\delta S = S[\bar{x} + \delta x] - S[\bar{x}] = 0$$

Derive the classical lagrangian equation of motion by applying the principle of least action.

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0 \tag{2}$$

Answer:

$$\begin{aligned} S[x + \delta x] &= \int_{t_a}^{t_b} L(\dot{x} + \delta \dot{x}, x + \delta x, t) dt \\ &= \int_{t_a}^{t_b} \left[L(\dot{x}, x, t) + \delta \dot{x} \frac{\partial L}{\partial \dot{x}} + \delta x \frac{\partial L}{\partial x} \right] dt \\ &= S[x] + \int_{t_a}^{t_b} \left[\delta \dot{x} \frac{\partial L}{\partial \dot{x}} + \delta x \frac{\partial L}{\partial x} \right] dt \end{aligned}$$

Upon integration by parts, the variation in S becomes

$$\delta S = \left[\delta x \frac{\partial L}{\partial \dot{x}}\right]_{t_a}^{t_b} - \int_{t_a}^{t_b} \delta x \left[\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x}\right] dt$$

Since $\delta x(t)$ is zero at the end points, the first term on the right-hand side of the equation is zero. Between the end points $\delta x(t)$ can take on any arbitrary value. Thus the extremum is that curve along which the following condition is always satisfied:

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

1.3 Exercise (2 pts)

Derive Newton's second law from the classical Lagrangian equation of motion.

Answer:

$$L = \frac{1}{2}m\dot{x}^2 - V(x)\frac{\partial L}{\partial t} = m\dot{x}$$

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

$$\frac{d}{dt}(m\dot{x}) + \frac{\partial V}{\partial x} = 0$$

$$m\ddot{x} - F(x) = 0$$

1.4 Exercise (2 pts)

Find the classical action of a free particle of mass m (without any external force). Given that the $x(t_a) = x_a$ and $x(t_b) = x_b$.

Answer: $m\ddot{x} = 0,\ x(t) = at + c$, where a, c are constants. Using boundany conditions:

$$\begin{cases} x_a = x(t_a) = at_a + c \\ x_b = x(t_b) = at_b + c \end{cases}$$

$$\Rightarrow \begin{cases} a = \frac{x_b - X_a}{t_b - t_a} \\ c = \frac{x_b t_a - x_a t_b}{t_a - t_b} \end{cases}$$

$$
\begin{aligned}
\implies S_{Cl} &= \int \mathcal{L} dt \\
&= \frac{1}{2} m \int \dot{x}^2 dt \\
&= \frac{1}{2} m \int_{t_h}^{t_l} a^2 dt
\end{aligned}
$$

1.5 Exercise (3 pts)

Consider a one-dimensional closed system, in which the the lagrangian does not depend explicitly on time.

$$\frac{\partial L}{\partial t} = 0 \tag{3}$$

Then, the total differential of lagrangian will be

$$\frac{dL}{dt} = \frac{\partial L}{\partial x}\dot{x} + \frac{\partial L}{\partial \dot{x}}\ddot{x} \tag{4}$$

Show that the Hamiltonian

$$H = \dot{x}\frac{\partial L}{\partial \dot{x}} - L \tag{5}$$

does not change with time.

Hence, show that if the potential energy does not depend on velocity or time explicitly, the Hamiltonian equals the sum of kinetic and potential energy.

$$H = \frac{p^2}{2m} + V(x) \tag{6}$$

Answer:

$$\frac{dH}{dt} = \ddot{x}\frac{\partial L}{\partial \dot{x}} + \dot{x}\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{dL}{dt}$$

$$\frac{dH}{dt} = \ddot{x}\frac{\partial L}{\partial \dot{x}} + \dot{x}\frac{\partial L}{\partial x} - \frac{dL}{dt} = 0$$

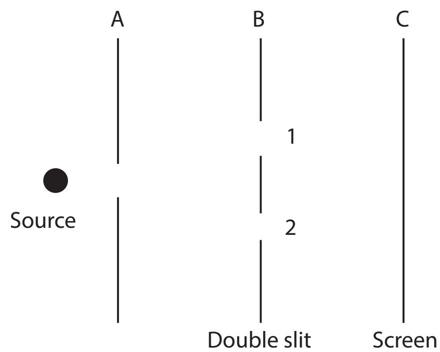
$$\frac{\partial L}{\partial x} = m\dot{x}$$

$$H = m\dot{x}^2 - \frac{1}{2}m\dot{x}^2 + V(x) = \frac{1}{2}m\dot{x}^2 + V(x) = \frac{p^2}{2m} + V(x)$$

2 Path-integral in quantum mechanics

2.1 Classical Mechanics vs Quantum Mechanics

One of the most important experiments showing the differences between classical and quantum mechanics is the double slit experiment.
Consider a source S of electrons (e^-) with identical energy. Electrons pass through a single slit and then a double slit and hit the screen.



On the screen C, the chance (probability density) of e^- hitting at a particular position x is measured as $P(x)$ when both slits 1 and 2 are opened, where x is some position on C.
The chance of e^- hitting at x is measured as $P_1(x)$ when only slit 1 is opened.
The chance of e^- hitting at x is measured as $P_2(x)$ when only slit 2 is opened.

In classical physics, $P(x) = P_1(x) + P_2(x)$. In quantum mechanics, $P(x) = P_1(x) + P_2(x) + P_{in}(x)$, where $P_{in}(x)$ is the interference term.

To account for the extra term, we postulate that

$$P(x) = |\Phi(x)|^2 \tag{7}$$

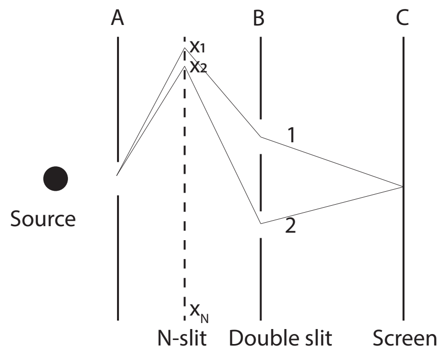
where $\Phi(x)$ is a complex number called the probability amplitude. Let Φ_1 and Φ_2 be the amplitudes when electrons pass through slit 1 and 2 respectively. The principle of superposition says the probability amplitudes add up linearly

$$\Phi = \Phi_1 + \Phi_2 \text{ and } P = |\Phi_1|^2 + |\Phi_2|^2 + 2\,\mathrm{Re}(\Phi_1^* \Phi_2) \tag{8}$$

Now let's examine this amplitude more carefully:

2.2 Intuitive approach to the path integral formalism

Insert an N-slit in between A and B.



Applying principle of superposition, we have

$$\Phi = \sum_{i=1}^{N} \sum_{m=1,2} \Phi(x_i, m) \tag{9}$$

Taking $N \to \infty$,

$$\Phi = \sum_{m=1,2} \int dx_i \Phi(x_i, m) \tag{10}$$

In general, we postulate that

$$\Phi = U(x_f, t_f; x_i, t_i) = \sum_{\gamma} \Phi(\gamma) = C \sum_{\gamma} e^{iS[\gamma]/\hbar} \tag{11}$$

where $\{\gamma\}$ is the set of all trajectories which satisfies $x(t_i) = x_i$ and $x(t_f) = x_f$ C is a constant to be determined. We want classical trajectories to describe the motion in the formal limit $\hbar \to 0$.

2.2.1 Exercise (1 pt)

Show that action has the same dimension as $\hbar$.

Answer: Obvious from the formula.

The classical limit means $S \gg \hbar$. If $\frac{S}{\hbar}$ is very large, the classical extremum path $\bar{x}(t)$ is the path where the phase becomes stationary,

$$\frac{\delta}{\delta x(t)} \left(\text{phase}[x(t)]\right)|_{\bar{x}(t)} = 0 \tag{12}$$

phase $= S/\hbar$. We can write it as:

$$\frac{\delta}{\delta x(t)} \left(S[x(t)]\right)|_{\bar{x}(t)} = 0 \tag{13}$$

The neighboring paths have similar phases as the extremum path, since the first order correction $\delta S = S[\bar{x} + \delta x] - S[\bar{x}] = 0$, so the contributions around the classical extremum path add up.
The other paths that are far from the classical extremum have strongly oscillating phases, so they interfere destructively and cancel each other.
When $\hbar \to 0$, the phases oscillate so violently that all paths that are not classical cancel each other's contributions, and only the classical path's contribution remains. This is the origin of the principle of least action.

2.2.2 Exercise (2 pts)

Consider an alpha particle travelling in air. Take the distance travelled be the average range in air. Compare the order of magnitude of the classical action and $\hbar$. Determine whether we should apply quantum mechanics in this case.

Answer: $S \approx \frac{1}{2}mv^2t = \frac{1}{2}mvd \approx 10^-27 \times 10^7 \times 10^-2 \approx 10^-22$(or similar order of magnitude)$\gg \hbar = 1.05 \times 10^{-34}$.
We can apply classical mechanics.

2.3 Postulates of Path Integral Formalism of Quantum Mechanics[1]

Postulate 1: The probability $P(b,a)$ of a particle moving from point a to point b is the square of the absolute value of a complex transition function $|U(b,a)|^2$

$$P(b,a) = |U(b,a)|^2 \tag{14}$$

Postulate 2: The transition function (also called the propagation amplitude) $U(b,a)$ is given by the sum of a phase factor $e^{\frac{iS}{\hbar}}$, where S is the action, taken over all possible paths from a to b.

$$U(b,a) = \sum_{\text{all paths}} \phi[x(t)] = \sum_{\text{all paths}} Ce^{iS/\hbar} \tag{15}$$

where the normalising constant C is independent of paths and can be determined by

$$U(b,a) = \sum_{\text{all paths}} U(b,c)U(c,a) \tag{16}$$

where we sum over all intermediate point c connecting a and b. If there are infinite intermediate point c connecting a and b, the equation can be written as:

$$U(b,a) = \int U(b,c)U(c,a)dx_c \tag{17}$$

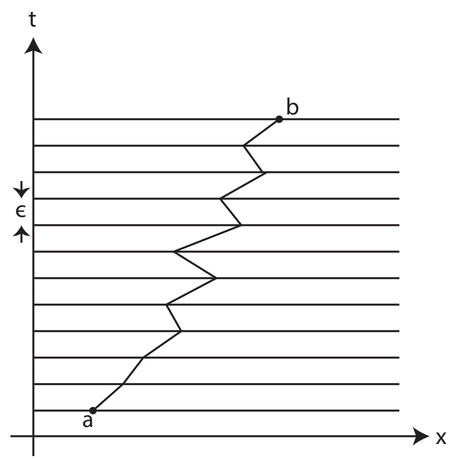
[1]This set of postulates is far from complete. See section 2.7 for more postulates. The only change from the usual Schrödinger picture's postulates is that the time evolution of wave function follows path integral representation, not Schrödinger's function.

2.3.1 Exercise (1 pts)

Discuss the physical meaning of the constancy of C in all different paths.
Answer: All paths matter! All paths contribute equally in calculation of the amplitude.

2.4 Riemann's sum

Let's discuss the equation in more detail. Discretize the time interval $T = t_b - t_a$ into N equal intervals of time ϵ. $N\epsilon = t_b - t_a$
$t_a = t_0$ and $x(t_a) = x_a = x_0$
$t_b = t_N$ and $x(t_b) = x_b = x_N$
$x(t_i) = x_i$



Then we can get

$$U(b,a) = \sum_{\text{all paths}} \phi[x(t)] = \text{constant} \int ... \int \int \phi[x(t)] dx_1 dx_2 ... dx_{N-1} \tag{18}$$

Remember that the initial point and final point are fixed, so we do not integrate over x_0 and x_N. Take $N \to \infty$ (the equal time interval $\epsilon \to 0$); we have

$$U(b,a) = \lim_{\epsilon \to 0} \frac{1}{A} \int ... \int \int e^{(i/\hbar)S[x]} \frac{dx_1}{A} \frac{dx_2}{A} ... \frac{dx_{N-1}}{A} \tag{19}$$

where

$$S[x] = \int_{t_a}^{t_b} L(\dot{x}, x, t) dt \tag{20}$$

A is function of ϵ added to the equation to normalize the propagator.

In simplicity, we write the sum over all paths as a path integral.

$$U(b,a) = \int_a^b e^{(i/\hbar)S[x]} \mathcal{D}x(t) \tag{21}$$

The path integral is defined as

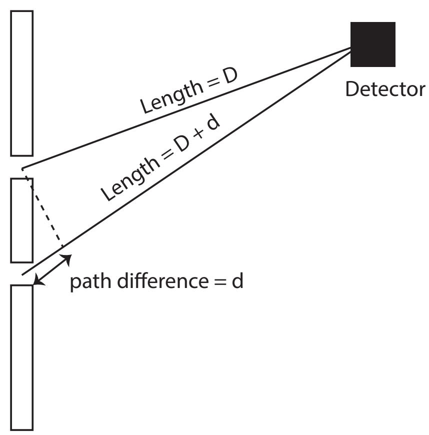
$$\int \mathcal{D}x = \frac{1}{A}\int ... \int\int \frac{dx_1}{A}\frac{dx_2}{A}...\frac{dx_{N-1}}{A} = \frac{1}{A}\prod_k \int \frac{dx_k}{A} \tag{22}$$

2.4.1 Exercise (1 pts)

Show your argument that A is function of ϵ.

Answer: Obviously, the infinitesimal displacement dx_i depends on ϵ s.t. $\epsilon \to 0$ implies that $dx_i \to 0$. If A does not tend to 0 when $\epsilon \to 0$, i.e. A depends on ϵ, the integral will become 0.

2.4.2 Exercise: Double slit interference of electrons (3 pts)



The distances from both slits to the detector are D and $D + d$ respectively. The action for either path is $(1/2)mv^2t$, which is the kinetic energy times time. Assume $d \ll D$ so that the speed of the electrons from both slits are similar $v_1 \approx v_2$. Show that the phase difference between these two paths $\approx 2\pi d/\lambda$, as expected, where λ is the de Broglie wavelength of the electron.

Answer: Remind that: similar speed does not mean same speed.
The two particles should reach the detector at the same time Δt so that they can interfere.
Let L_i be the distance from the slit to the detector
The action $S_i = \frac{1}{2}mv \times L_i = \frac{1}{2}m{L_i}^2/\Delta t$
de Broglie wavelength $\lambda = \frac{h}{p} = 2\pi\frac{\hbar}{mv}$
the phase difference $= \frac{1}{\hbar}(S_1 - S_2) = \frac{m}{2\hbar\Delta t}[(D+d)^2 - D^2] \approx \frac{m}{2\hbar\Delta t} \times 2Dd \approx \frac{mvd}{\hbar} = \frac{2\pi d}{\lambda}$

2.5 Wave function

$U(x_b, t_b; x_a, t_a)$ is the transition function or amplitude for a particle to reach a particular point in space and time from a particular initial point. It would also

be useful to define the amplitude to arrive a specific place without specifying the previous motion. The wave function $\psi(x,t)$ is defined as the total amplitude to arrive at (x,t).
Therefore, if the particle comes from a particular initial point (x_a,t_a), the amplitude from (x_a,t_a) to (x_b,t_b) = the amplitude at (x_b,t_b).

$$U(x_b,t_b;x_a,t_a) = \psi(x_b,t_b) \tag{23}$$

Generally, a particle can come from any initial point, so the wave function satisfies the integral equation:

$$\psi(x_b,t_b) = \int_{-\infty}^{\infty} U(x_b,t_b;x_c,t_c)\psi(x_c,t_c)dx_c \tag{24}$$

$|\psi(x,t)|^2$ is again the probability density to find the particle at (x,t).

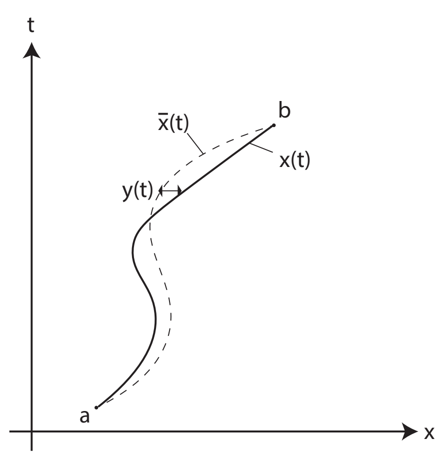
2.6 Technique in doing Path Integral

We want to determine

$$U(b,a) = \int_a^b \exp(\frac{i}{\hbar}\int_{t_a}^{t_b} L(\dot{x},x,t)dt)\mathcal{D}x(t) \tag{25}$$

over all paths from (x_a,t_a) to (x_b,t_b). Let $\bar{x}(t)$ be the classical path which is the extremum for the action.

$$S_{cl}[b,a] = S[\bar{x}(t)] \tag{26}$$



For a arbitrary path, we can write it as

$$x(t) = \bar{x}(t) + y(t) \tag{27}$$

where $y(t)$ is the deviation from the classical path. Since the end points and classical path is fixed, $y(t_a) = y(t_b) = 0$ and $\int \mathcal{D}x(t) = \int \mathcal{D}y(t)$
From equation (24),

$$\psi(x_b, t_b) = \int_{-\infty}^{\infty} U(x_b, t_b; x_a, t_a)\psi(x_a, t_a)dx_a \tag{28}$$

2.6.1 Exercise I (2 pt)

Let t_b differs by an infinitesimal interval ϵ from t_a, i.e. $t_b = t_a + \epsilon$.
Also, consider $x_b = x_a - \eta$.
Since the interval is infinitesimally small, we can take the speed be η/ϵ, the potential energy be $V(x_b + \eta/2)$ during the interval ϵ. $\int_{t_a}^{t_b} f(t)dt \approx f(t_a)\epsilon$. Show the following equation holds:

$$\psi(x_b, t_a+\epsilon) = \frac{1}{A}\int_{-\infty}^{\infty} \exp\left\{\frac{im\eta^2}{2\hbar\epsilon}\right\} \times \exp\left\{-\frac{i}{\hbar}\epsilon V\left(x_b + \frac{\eta}{2}, t_a\right)\right\}\psi(x_b + \eta, t_a)d\eta \tag{29}$$

Answer: When ϵ is small,

$$\psi(x_b, t_a + \epsilon) = \frac{1}{A}\int_{-\infty}^{\infty} \exp\left\{\frac{iS[b, a]}{\hbar}\right\} \times\psi(x_b + \eta, t_a)d\eta \tag{S2}$$

where the action is

$$S[b, a] = \left(\frac{m(\Delta x)^2}{2(\Delta t)^2} - V\left(\frac{x_b + x_a}{2}, t_a\right)\right)\Delta t = \frac{m\eta^2}{2\epsilon} - \epsilon V\left(x_b + \frac{\eta}{2}, t_a\right) \tag{S3}$$

To first order approximation, it does not matter whether we pick $V\left(x_b + \frac{\eta}{2}, t_a\right)$, or $V\left(x_b + \frac{\eta}{2}, t_a + \epsilon\right)$: it is ϵV appearing in the action and the above changes in the argument of V would be second order and can be ignored in the limit ϵ is small.

2.6.2 Exercise II (4 pt)

If η is large, the first exponential will oscillate very rapidly and give a small value of the integral. Hence, only if η is small enough, the first exponential will contribute the most in the integral.
Expanding the terms in the integral, we have

$$\psi(x_b, t_a) + \epsilon\frac{\partial\psi}{\partial t_a} = \frac{1}{A}\int_{-\infty}^{\infty} \exp\left\{\frac{im\eta^2}{2\hbar\epsilon}\right\} \times [1 - \frac{i}{\hbar}\epsilon V(x_b, t_a)][\psi(x_b, t_a) + \eta\frac{\partial\psi}{\partial x_b}]d\eta \tag{30}$$

By comparing the term of $\psi(x_b, t_a)$ on both sides, show that $A = \sqrt{\frac{2\pi i\hbar\epsilon}{m}}$
Hint: $\int_{-\infty}^{\infty} e^{-x^2}dx = \sqrt{\pi}$

Answer: Focusing on the largest term on both sides (the term $\eta\frac{\partial\psi}{\partial x_b}$ is integrated to zero because it is an odd function of η):

$$\psi(x_b, t_a) = \frac{1}{A}\int_{-\infty}^{\infty} \exp\left\{\frac{im\eta^2}{2\hbar\epsilon}\right\} \times \psi(x_b, t_a) d\eta = \frac{1}{A}\sqrt{\frac{2\pi\hbar\epsilon}{-im}}\psi(x_b, t_a) \tag{S4}$$

Therefore

$$A = \sqrt{\frac{2\pi i\hbar\epsilon}{m}} \tag{S5}$$

2.7 Basics of Quantum mechanics

2.7.1 Dirac Notation: Bra & Ket

Physical state of a system is represented in quantum mechanics by ket (vectors) in a complex Hilbert space[2].
Dirac denoted the state vector ψ by a ket $|\psi\rangle$.
Dirac denoted the Hermitian conjugate of a ket by a bra vector $\langle\psi|$. Hermitian conjugate means conjugate and transpose.
For each ket vector $|\psi\rangle$, there exists a unique bra vector $\langle\psi|$, vice versa.
For example, if the Hilbert space is n-dimensional,

$$|\psi\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \cdots \\ a_n \end{pmatrix}, \quad \langle\psi| = (|\psi\rangle)^+ = (a_1^*, a_2^*, \cdots, a_n^*) \tag{31}$$

where $a_i \in \mathbb{C}$, * means complex conjugation and $^+$ is Hermitian conjugate.

2.7.2 Inner product

The inner product of bra and ket vectors is denoted as $\langle\phi|\psi\rangle$, which is a complex number. For example, suppose

$$|\psi\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \cdots \\ a_n \end{pmatrix}, \quad |\phi\rangle = \begin{pmatrix} b_1 \\ b_2 \\ \cdots \\ b_n \end{pmatrix}, \quad \text{then} \quad \langle\phi|\psi\rangle = \sum_{i=1}^{n} b_i^* a_i \tag{32}$$

which is the same as matrix multiplication between $1 \times n$ matrix $\langle\phi|$ and $n \times 1$ matrix $|\psi\rangle$. Whenever we write a state $|\psi\rangle$, *we always assume the state is normalized:* $\langle\psi|\psi\rangle = 1$.

[2]Think of a Hilbert space as a vector space, so every state is represented by a complex vector.

2.7.3 Operator

Operator in quantum mechanics is a linear function that maps one state to another.
A state vector $|\psi\rangle$ is said to be an eigenvector of an operator $\hat{A}$ if

$$\hat{A}|\psi\rangle = a|\psi\rangle \tag{33}$$

where $a \in \mathbb{C}$ is called eigenvalue. We always write a 'hat' above a letter (in this case, A) to represent an operator $\hat{A}$.

2.7.4 Position Representation

The *value* of a state $|\psi\rangle$ at position x is given by

$$\psi(x) = \langle x|\psi\rangle \tag{34}$$

where $\psi(x)$ is a complex number and $|x\rangle$ is a ket vector that represents the position x in Hilbert space. Define $\hat{x}$ to be the position operator s.t. $\hat{x}|x\rangle = x|x\rangle$, where x is the eigenvalue when $\hat{x}$ operates on $|x\rangle$. $|x\rangle$ is an eigenvector of $\hat{x}$. The set of all position eigenstates, $\{|x\rangle\}$, form a orthonormal basis for the Hilbert space:

$$\int dx|x\rangle\langle x| = \hat{I}, \quad \langle x|y\rangle = \delta(x-y) \tag{35}$$

where $\hat{I}$ is the identity operator and δ is the Dirac Delta function (see next). Therefore

$$\int dx|x\rangle\langle x|\psi\rangle = \hat{I}|\psi\rangle = |\psi\rangle \tag{36}$$

for any state $|\psi\rangle$.

The Dirac delta function, $\delta(x)$, is defined as:

$$\delta(x) = \left\{ \begin{array}{ll} 0, & \text{if } x \neq 0 \\ \infty, & \text{if } x = 0 \end{array} \right\}, \text{ with } \int_{-\infty}^{+\infty} \delta(x)dx = 1.$$

It is an infinitely high, infinitesimally narrow spike at the origin, whose area is 1. It is a generalization to continuous variable of the discrete Kronecker delta function:

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \tag{37}$$

You will need the following identity:

$$\int_{-\infty}^{+\infty} f(x)\delta(x-a)dx = f(a)\int_{-\infty}^{+\infty} \delta(x-a)dx = f(a) \tag{38}$$

3 Propagator for a free particle

We want to calculate the propagator for a free particle moving in one dimension, that is a particle moving without being subjected to any potential. Recall from eq. 21 that

$$U\left(x_1, t; x_0, t_0\right) = \int_{x(t_0)=x_0}^{x(t)=x_1} \mathcal{D}x \ \exp\left[\frac{i}{\hbar}\int_{t_0}^{t} dt\mathcal{L}\right] \tag{39}$$

We now need to calculate the action for our particle. The possible trajectory $x(t)$ will be considered between (x_a, t_a) and (x_b, t_b). We will divide the path in N discrete small paths of equal duration, before taking the limit $N \to \infty$. Then we will have $\Delta t = \frac{t_b - t_a}{N}$ and the intermediary points will have the coordinates $(x_1, t_1), (x_2, t_2), ..., (x_{N-1}, t_{N-1})$.

3.1 Exercise (3 pts)

Prove that the action S_i corresponding to the i-th segment of the path is $\frac{m}{2\Delta t}(x_i - x_{i-1})^2$. Consider the velocity to be constant during this motion.

Answer: We simply apply the definition of action:

$$S_i = \int_{t_{i-1}}^{t_i} \frac{m}{2}\dot{x}(t)^2 dt = \frac{m}{2}\left(\frac{x_i - x_{i-1}}{t_i - t_{i-1}}\right)^2 (t_i - t_{i-1}) = \frac{m}{2\Delta t}\left(x_i - x_{i-1}\right)^2 \tag{S6}$$

Now we require to describe each path between starting and end points, so for each time interval we can vary x_i over the whole real domain. The sum of all contributions will be:

$$U(x_N, t_N; x_0, t_0) = C(t) \int_{-\infty}^{+\infty} ... \int_{-\infty}^{+\infty} \exp\Big[\frac{i}{\hbar}S\Big] dx_1 ... dx_n \tag{40}$$

Here $C(n)$ is the normalization constant, depending only on $t_N - t_0 = t_b - t_a$.

3.2 Exercise (6 pts)

Calculate the integral presented above over x_1 and x_2, then write a recurrence that allows us to calculate all integrals. Normalize your result to obtain the propagator $U(x, t; x_0)$.

Hint: Ignore the constants appearing during successive integration, as you only have to normalize the final result.

Answer: The calculation is carried out as follows. Notice first that

$$\begin{gathered}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{2/2} \int_{-\infty}^{\infty} \exp\left\{\frac{im}{2\hbar\Delta t}\left[\left(x_2 - x_1\right)^2 + \left(x_1 - x_0\right)^2\right]\right\} dx_1 = \\ \left(\frac{m}{2\pi i\hbar \cdot 2\Delta t}\right)^{1/2} \exp\left\{\frac{im}{2\hbar \cdot 2\Delta t}\left(x_2 - x_0\right)^2\right\}\end{gathered} \tag{S7}$$

Next we multiply this result by $\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2} \exp\left\{\frac{im}{2\hbar\Delta t}\left(x_3 - x_2\right)^2\right\}$ and integrate again, this time over x_2. The result is similar to that of the previous equation, except that $\left(x_2 - x_0\right)^2$ becomes $\left(x_3 - x_0\right)^2$ and the expression $2\Delta t$ is replaced by $3\Delta t$ in two places. Thus we get

$$\left(\frac{m}{2\pi i\hbar \cdot 3\Delta t}\right)^{1/2} \exp\left\{\frac{im}{2\hbar \cdot 3\Delta t}\left(x_3 - x_0\right)^2\right\} \tag{S8}$$

In this way a recursion process is established which, after $n-1$ steps, gives

$$\left(\frac{m}{2\pi i\hbar \cdot n\Delta t}\right)^{1/2} \exp\left\{\frac{im}{2\hbar \cdot n\Delta t}\left(x_n - x_0\right)^2\right\} \tag{S9}$$

Now we consider that $n\Delta t = t_N - t_0 = t_b - t_a$ and achieve the desired result.

4 Deriving Schrödinger equation from path integrals

We have investigated how quantum mechanics can be expressed in terms of path integrals. Now we seek to show that Schrödinger's equation, one of the very foundations of quantum mechanics, can be deduced from path integrals. Consider a one dimensional system characterized by a potential energy $V(x)$, an initial state $|\psi(t_0)\rangle$, and infinitesimal increments δx and δt. The new state can be described as:

$$\psi(x,t) = \int dx_0 \; U\left(x,t;x_0,t_0\right) \psi(x_0,t_0) \tag{41}$$

Let us begin by calculating the propagator U. Again, we will assume for the small time interval we study the velocity to be $\dot{x} = \frac{\delta x}{\delta t}$ and average position as $x_0 + \frac{\delta x}{2}$.

4.1 Exercise (3 pts)

Derive an expression for the action of this system and its propagator up to a normalization constant depending on δt.

Answer:

$$L = \frac{m}{2}\dot{x}(t)^2 - V(x(t)) \tag{S10}$$

$$U\left(x,t;x_0,t_0\right) = A(\delta t)\exp\left[\frac{i}{\hbar}\int_0^{\alpha} dt \left(\frac{m}{2}\dot{x}(t)^2 - V(x(t))\right)\right] \tag{S11}$$

Since we used infinitesimal increments in time and coordinate, we can expand the propagator and potential using these infinitesimal increments.

4.2 Exercise (5 pts)

Write the first-order expansion in δx and δt for $U(x_0 + \delta x, t_0 + \delta t; x_0)$ and $V(x_0 + \frac{\delta x}{2})$.

Answer:

$$U\left(x,t;x_0,t_0\right) \approx A(\delta t)\exp\left[\frac{i}{\hbar}\left(\frac{m}{2\delta t}\delta x^2 - V\left(x_0 + \frac{\delta x}{2}\right)\delta t\right)\right] \tag{S12}$$

$$\frac{i\delta t}{\hbar}\exp\left[-V\left(x_0 + \frac{\delta x}{2}\right)\right] = 1 - \frac{i\delta t}{\hbar}V\left(x_0 + \frac{\delta x}{2}\right) + \dots \tag{S13}$$

$$V\left(x_0 + \frac{\delta x}{2}\right) = V\left(x_0\right) + \frac{\delta x}{2}\frac{d}{d\delta x}V\left(x_0\right) + \dots \tag{S14}$$

We also need to expand the ket in the integrand:

$$\psi(x_0 + \delta x, t) = \psi(x_0,t) + \frac{\partial \psi(x_0,t)}{\partial x}\delta x + \frac{1}{2}\frac{\partial^2 \psi(x_0,t)}{\partial x^2}(\delta x)^2 \tag{42}$$

The second term of this expansion is odd, so we can disregard it when integrating on the whole real axis.

4.3 Exercise (4 pts)

Replace the quantities in the path integral with their expansions and obtain Schrödinger's equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t_0) = \Big(V(x_0) - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Big)\psi(x_0,t_0) \tag{43}$$

Hint: Obtain the time derivative by taking the limit for δt.

Answer:

$$\begin{aligned}\psi\left(x,t_0+\delta t\right) =& A(\delta t)\left[1-\frac{i\delta t}{\hbar}V\left(x_0\right)\right]\int_{-\infty}^{\infty} d(\delta x)\left[\psi(x_0,t)+\frac{1}{2}(\delta x)^2\frac{d^2\psi(x_0,t)}{dx^2}\right]\\ &\exp\left[\frac{i}{\hbar}\frac{m}{2\delta t}(\delta x)^2\right]\end{aligned} \tag{S15}$$

It is straightforward to evaluate this Gaussian. Integrating, and keeping the first order terms in the infinitesimals gives

$$\psi\left(x_0,t_0+\delta t\right) = A(\delta t)\sqrt{\frac{2\hbar\pi\delta t}{im}}\left[1-\frac{i\delta t}{\hbar}V\left(x_0\right)+\frac{\hbar\delta t}{2mi}\frac{d^2}{dx^2}\right]\psi\left(x_0,t_0\right) \tag{S16}$$

For small δt, we see that the first term on the right must equal the expression on the left, and that the normalization constant is necessarily $A(\delta t) = \sqrt{\frac{m}{2\pi hi\delta t}}$. To recover the time derivative, we can rearrange S16 and take the limit as $\delta t \to 0$ of $i\left[\psi\left(x,t_0+\delta t\right)-\psi\left(x,t_0\right)\right]/(\hbar\delta t)$.

Other expressions of Schrödinger's equation characterizing different systems can also be obtained from path integrals following a similar method.

We define the time-independent *Hamiltonian* operator as:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}), \quad \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{44}$$

The Hamiltonian can be classically understood as the energy of a particle. In quantum mechanics we have to think of it as an operator that acts on a ket. Schrödinger's equation becomes:

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle \tag{45}$$

We now wish to show the first equality in the following expression:

$$U\left(x_1,t;x_0,t_0\right) = \left\langle x_1\left|e^{-i\hat{H}(t-t_0)/\hbar}\right|x_0\right\rangle = \int_{x(t_0)=x_0}^{x(t)=x_1}\mathcal{D}x\ \exp\left[\frac{i}{\hbar}\int_{t_0}^{t}dt\mathcal{L}\right] \tag{46}$$

As our Hamiltonian is constant in time, we can write a solution to the equation as[3]:

$$|\psi(t)\rangle = e^{-i\hat{H}(t-t_0)/\hbar}|\psi(t_0)\rangle \tag{47}$$

By multiplying this equation with $\langle x|$:

$$\psi(x,t) = \langle x|\psi(t)\rangle = \langle x|e^{-i\hat{H}(t-t_0)/\hbar}|\psi(t_0)\rangle \tag{48}$$

Now we can insert here an identity operator of the form $\int dx_0|x_0\rangle\langle x_0| = \hat{\mathrm{I}}$

$$\psi(x,t) = \langle x|\psi(t)\rangle = \langle x|e^{-i\hat{H}(t-t_0)/\hbar}\int dx_0|x_0\rangle\langle x_0|\psi(t_0)\rangle \tag{49}$$

We recognize in this equation $\psi(x_0,t_0) = \langle x_0|\psi(t_0)\rangle$. Now we can rewrite the equation as:

$$\psi(x,t) = \int dx_0\langle x|e^{-i\hat{H}(t-t_0)/\hbar}|x_0\rangle\psi(x_0,t_0) = \int dx_0 U(x,t,x_0,t_0)\psi(x_0,t_0) \tag{50}$$

[3]This solution can be obtained by performing a separation of variables in Schrödinger's equation, namely $\psi(x,t) = \psi(x)\phi(t)$

5 Propagator for harmonic oscillator

As another example of the computation of Path Integral, consider the propagator for a forced harmonic oscillator. It follows the equation of motion

$$\ddot{x} + w^2 x = \frac{f(t)}{m} \tag{51}$$

The general solution is $x = x_c + x_p$, where x_c is the solution of the homogeneous equation

$$\ddot{x} + \omega^2 x = 0 \tag{52}$$

The homogeneous solution is of the form

$$x_c = A\sin(\omega t) + B\cos(\omega t) \tag{53}$$

One particular solution, x_p, that satisfies the inhomogeneous equation 51 has the form:

$$x_{\mathrm{p}}(t) = \frac{1}{m\omega}\frac{\sin\omega\,(t_a - t)}{\sin\omega\,(t_b - t_a)}\int_{t_a}^{t_b}\sin\omega(t_b - t')f(t')\mathrm{d}t' + \frac{1}{m\omega}\int_{t_a}^{t}\sin\omega(t - t')f(t')\mathrm{d}t' \tag{54}$$

The final solution is a sum of these two $x = x_c + x_p$. After some calculations, the classical action for such system is

$$\begin{aligned} S_{\mathrm{cl}} = & \frac{m\omega}{2\sin\omega T}\Big[\cos\omega T\left(x_b^2 + x_a^2\right) - 2x_b x_a \\ & + \frac{2x_a}{m\omega}\int_{t_a}^{t_b}\sin(\omega\,(t_b - t))f(t)\mathrm{d}t + \frac{2x_b}{m\omega}\int_{t_a}^{t_b}\sin(\omega\,(t - t_a))f(t)\mathrm{d}t \\ & - \frac{2}{m^2\omega^2}\int_{t_a}^{t_b}\int_{t_a}^{t}\sin(\omega\,(t_b - t))\sin(\omega\,(t' - t_a))f\,(t')\,f(t)\mathrm{d}t'\mathrm{d}t\Big] \end{aligned} \tag{55}$$

5.1 Exercise (2 pts)

Prove that x_c and x_p are homogeneous and particular solutions to equation 51. Using the boundary conditions $x(t_a) = x_a$ and $x(t_b) = x_b$ obtain the equations for A and B.

Answer: [4]

$$\ddot{x}_c = -A\omega^2\sin(\omega t) - B\omega^2\cos(\omega t) = -\omega^2 x_c$$

Using the equation

$$f(x) = \int_{s(x)}^{g(x)} h(x,t)dt$$

$$\frac{df}{dx} = \int_{s(x)}^{g(x)}\partial_x h(x,t)dt + h(x,g(x))\frac{dg}{dx} - h(x,s(x))\frac{ds}{dx},$$

[4]This solution is copied from team AceD's answers.

and setting $x = t, t = t', h(t,t') = \sin(\omega(t-t')) f(t'), g(t) = t$, and $s(t) = t_a$ in the formula, we get

$$\begin{aligned}
\dot{x}_p = &-\frac{1}{m}\frac{\cos(\omega(t_a - t))}{\sin(\omega(t_b - t_a))}\int_{t_a}^{t_b} \sin(\omega(t_b - t')) f(t')\, dt' \\
&+ \frac{1}{m\omega}\left[\int_{t_a}^{t} \omega\cos(\omega(t - t')) f(t')\, dt' + \sin(\omega(t-t))f(t)\right] \\
= &-\frac{1}{m}\frac{\cos(\omega(t_a - t))}{\sin(\omega(t_b - t_a))}\int_{t_a}^{t_b} \sin(\omega(t_b - t')) f(t')\, dt' + \frac{1}{m}\int_{t_a}^{t} \cos(\omega(t - t')) f(t')\, dt'
\end{aligned}$$

Using the formula again, we get

$$\begin{aligned}
\ddot{x}_p = &-\frac{1}{m}\frac{\sin(\omega(t_a - t))}{\sin(\omega(t_b - t_a))}\int_{t_a}^{t_b} \sin(\omega(t_b - t')) f(t')\, dt' \\
&- \frac{1}{m}\left[\int_{t_a}^{t} \omega\sin(\omega(t - t')) f(t')\, dt' + \cos(\omega(t-t))f(t)\right] \\
= &-\frac{1}{m}\frac{\sin(\omega(t_a - t))}{\sin(\omega(t_b - t_a))}\int_{t_a}^{t_b} \sin(\omega(t_b - t')) f(t')\, dt' \\
&- \frac{1}{m}\int_{t_a}^{t} \omega\sin(\omega(t - t')) f(t')\, dt' + \frac{f(t)}{m} \\
= &-\omega^2 x_p + \frac{f(t)}{m}
\end{aligned}$$

At t_a we have

$$x(t_a) = A\sin(\omega t_a) + B\cos(\omega t_a).$$

The factors in x_p are zero at this time because $\sin(\omega(t_a - t))$ will be zero and the bounds of the second integral will match and the integral will vanish. At t_b we have

$$\begin{aligned}
x(t_b) = &A\sin(\omega t_b) + B\cos(\omega t_b) + \frac{1}{m\omega}\frac{\sin(\omega(t_a - t_b))}{\sin(\omega(t_b - t_a))}\int_{t_a}^{t_b} \sin(\omega(t_b - t')) f(t')\, dt' \\
&+ \frac{1}{m\omega}\int_{t_a}^{t_b} \sin(\omega(t_b - t')) f(t')\, dt' \\
= &A\sin(\omega t_b) + B\cos(\omega t_b) - \frac{1}{m\omega}\int_{t_a}^{t_b} \sin(\omega(t_b - t')) f(t')\, dt' \\
&+ \frac{1}{m\omega}\int_{t_a}^{t_b} \sin(\omega(t_b - t')) f(t')\, dt' \\
= &A\sin(\omega t_b) + B\cos(\omega t_b).
\end{aligned}$$

Since $x(t_a) = x_a$ and $x(t_b) = x_b$, we can solve for A and B in terms of these variables:

$$\begin{aligned}
x_a\sin(\omega t_b) &= A\sin(\omega t_a)\sin(\omega t_b) + B\cos(\omega t_a)\sin(\omega t_b) \\
x_b\sin(\omega t_a) &= A\sin(\omega t_a)\sin(\omega t_b) + B\sin(\omega t_a)\cos(\omega t_b).
\end{aligned}$$

Subtracting these equations and factoring out B yields

$$B = \frac{x_a \sin(\omega t_b) - x_b \sin(\omega t_a)}{\cos(\omega t_a)\sin(\omega t_b) - \cos(\omega t_b)\sin(\omega t_a)}.$$

Doing the same for A yields

$$A = \frac{x_a \cos(\omega t_b) - x_b \cos(\omega t_a)}{\cos(\omega t_b)\sin(\omega t_a) - \cos(\omega t_a)\sin(\omega t_b)}$$

5.2 Exercise (5 pts)

Show that for $f(t) = 0$ resulting kernel is

$$K = F(T)\exp\left\{\frac{im\omega}{2\hbar \sin\omega T}[(x_b^2 + x_a^2)\cos\omega T - 2x_b x_a]\right\} \tag{56}$$

where $T = t_b - t_a$ and multiplicative function $F(T)$ is defined as:

$$F(T) = \left(\frac{m\omega}{2\pi i\hbar \sin\omega T}\right)^{1/2} \tag{57}$$

You don't have to prove this multiplicative factor until exercise 5.4, but you need to write down the path integral equation for this factor and shows that it only depends on T.

Answer: [5] Calculating the total energy of the system to get the action, we write

$$S_{cl} = \frac{m}{2}\int_0^T \left(\dot{x}^2 - \omega^2 x^2\right) dt = \frac{m}{2}\int_0^T v^2(t)dt - \frac{m}{2}\int_0^T \omega^2 x^2 dt$$

By evaluating integration by parts we get

$$\begin{aligned} S_{cl} &= \frac{m}{2}\left[[v(t)x(t)]_0^T - \int_0^T x(t)\ddot{x}(t)dt\right] - \frac{m}{2}\int_0^T \omega^2 x^2 dt \\ &= \frac{m}{2}\left[[v(t)x(t)]_0^T - \int_0^T x(t)\left(-\omega^2 x\right)dt\right] - \frac{m}{2}\int_0^T \omega^2 x^2 dt \\ &= \frac{m}{2}[v(T)x(T) - v(0)x(0)] \\ &= \frac{m}{2}[\dot{x}(T)x(T) - \dot{x}(0)x(0)] \end{aligned}$$

If we modify the homogeneous solution of forced harmonic oscillation given above by replacing the terms A and B by the equations we have found in the Exercise 1 , we get these equations:

$$\begin{aligned} x(t) &= A\sin\omega t + B\cos\omega t \\ &= \left(\frac{x_b - x_a\cos\omega T}{\sin\omega T}\right)\sin\omega t + x_a\cos\omega t \end{aligned}$$

[5] This solution is modified from team Boing's and team CEEUP's answers.

Now, we should find x and $\dot{x}$'s values at $t=0$ and T to substitute those values in our classical action equation:

$$\Rightarrow \dot{x}(T) = \left(\frac{x_b - x_a\cos\omega T}{\sin\omega T}\right)\omega\cos\omega t - x_a\omega\sin\omega t$$

$$\Rightarrow \dot{x}(0) = \left(\frac{x_b - x_a\cos\omega T}{\sin\omega T}\right)\omega, \quad x(T) = x_b, \quad x(0) = x_a$$

$$\begin{aligned}
S_{cl} &= \frac{m}{2}\left(\omega x_b\left(\frac{x_b - x_a\cos\omega T}{\sin\omega T}\right)\cos\omega T - x_a x_b\omega\sin\omega T - x_a\omega\left(\frac{x_b - x_a\cos\omega T}{\sin\omega T}\right)\right)\\
&= \frac{m\omega}{2}\left(\frac{x_b^2\cos\omega T - x_a x_b\cos\omega T^2 - x_a x_b\sin\omega T^2 - x_a x_b + x_a^2\cos\omega T^2}{\sin\omega T}\right)\\
&= \frac{m\omega}{2}\left(\frac{x_b^2\cos\omega T - 2x_a x_b + x_a^2\cos\omega T}{\sin\omega T}\right)\\
&= \frac{m\omega}{2\sin\omega T}\left[\left(x_a^2 + x_b^2\right)\cos\omega T - 2x_a x_b\right]
\end{aligned}$$

Now we consider a general path in the path integral. Let $\bar{x}$ be the classical path with action S_{cl} and $x = \bar{x} + y$. The action is

$$S = \int_{t_a}^{t_b}\frac{m}{2}\left(\dot{x}^2 - \omega^2 x^2\right) = \int_{t_a}^{t_b}\left(\frac{m}{2}\left(\dot{\bar{x}}^2 - \omega^2\bar{x}^2\right) + \frac{m}{2}\left(2\dot{\bar{x}}\dot{y} + \dot{y}^2 - \omega^2 y^2 - 2\omega^2\bar{x}y\right)\right)\mathrm{d}t$$

From the the equation of motion for the classical path $\bar{x}$ or the principle of least action, the linear terms in y will vanish. Measure does not change under translation: $\mathcal{D}x(t) = \mathcal{D}y(t)$, so

$$S = S_{cl} + \int_{t_a}^{t_b}\frac{m}{2}\left(\dot{y}^2 - \omega^2 y^2\right)\mathrm{d}t$$

$$\begin{aligned}
K(b,a) &= \int_a^b \exp\left\{\frac{i}{\hbar}S\right\}\mathcal{D}x(t)\\
&= \exp\left\{\frac{i}{\hbar}S_{cl}\right\}\int_0^0\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\frac{m}{2}\left(\dot{y}^2 - \omega^2 y^2\right)\mathrm{d}t\right\}\mathcal{D}y(t)
\end{aligned}$$

where the path integral has boundary condition $y(t_a) = y(t_b) = 0$. y does not depend on x_a and x_b, so the second term must only depend on t_a and t_b. But out theory has time-translational symmetry, so the second term can only be a function of $T = t_b - t_a$.

$$K(b,a) = F(T)\exp\left\{\frac{i}{\hbar}S_{cl}\right\}, \quad F(T) = \int_0^0\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\frac{m}{2}\left(\dot{y}^2 - \omega^2 y^2\right)\mathrm{d}t\right\}\mathcal{D}y(t)$$

5.3 Exercise (5 pts)

If the wave function of harmonic oscillator $(f(t) = 0)$ at time $t = 0$ is

$$\psi(x,0) = \exp\left\{-\frac{m\omega}{2\hbar}(x-a)^2\right\} \tag{58}$$

Show that

$$\psi(x,T) = \exp\left\{-\frac{i\omega T}{2} - \frac{m\omega}{2\hbar}[x^2 - 2axe^{-i\omega T} + a^2\cos(\omega T)e^{-i\omega T}]\right\} \tag{59}$$

Also, find the probability distribution $|\psi|^2$. You may need to normalize the wave function.

Answer: [6] Knowing the kernel for the harmonic oscillator potential, we can find the wave function at (x,T) making use of the very definition of a propagator:

$$\psi(x,T) = \int_{-\infty}^{\infty} K\left(x,T;x_0\right)\psi\left(x_0,0\right)dx_0$$

As we have been given that wave function at time $t=0$ is $\exp\left\{\frac{-m\omega}{2\hbar}(x-a)^2\right\}$, we can take the integral above in order to find $\psi(x,T)$.

$$\begin{aligned}\psi(x,T) =& \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\exp\left\{\frac{im\omega}{2\hbar\sin\omega T}x^2\cos\omega T\right\}\\ &\times\int_{-\infty}^{\infty}\exp\left\{\frac{m\omega}{2\hbar\sin\omega T}\left(ix_0^2\cos\omega T - 2ixx_0 - \sin\omega T\left(x_0-a\right)^2\right\}dx_0\end{aligned}$$

For the sake of convenience, let us first manipulate the argument of the exponential function inside the integral so that it will take a form that is easily integrable.

$$\begin{aligned}&ix_0^2\cos\omega T - 2ixx_0 - \sin\omega T\left(x_0-a\right)^2\\ =&ie^{i\omega T}\left(x_0^2 + 2ix_0(ix - a\sin\omega T)e^{-i\omega T}\right) - a^2\sin\omega T\\ =&ie^{i\omega T}\left(x_0 + i(ix - a\sin\omega T)e^{-i\omega T}\right)^2 + ie^{-i\omega T}(ix - a\sin\omega T)^2 - a^2\sin\omega T\end{aligned}$$

Second and third terms in the above expression can be taken out of the integral since they are independent of x_0. With only the first term inside, integral now takes the form a Gaussian integral solution of which is quite familiar.

$$\begin{aligned}\psi(x,T) &= \left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{\frac{1}{2}}\left(\frac{2\pi i\hbar\sin\omega T}{m\omega e^{i\omega T}}\right)^{\frac{1}{2}}\exp\left\{-\frac{m\omega}{2\hbar}\left(x^2 - 2axe^{-i\omega T} + a^2\cos\omega Te^{-i\omega T}\right)\right\}\\ &= \exp\left\{-\frac{i\omega T}{2} - \frac{m\omega}{2\hbar}\left(x^2 - 2axe^{-i\omega T} + a^2\cos\omega Te^{-i\omega T}\right)\right\}\end{aligned}$$

Now, we can find the probability distribution easily by first calculating the value $|\psi(x,T)|^2$ and then normalizing it. To do that, first let us define a function Φ which will make the calculations simpler. Let Φ be the argument of the exponent in the above expression for the wave function. Now we can decompose Φ into its real and imaginary parts, denoted by ϕ_r and ϕ_i respectively. Complex conjugate of the wave function will be equal to $\psi^* = \exp\left\{\phi_r - i\phi_i\right\}$. Then,

$$|\psi(x,T)|^2 = \psi\psi^* = \exp\left\{2\phi_r\right\} = \exp\{2\,\mathrm{Re}\{\Phi\}\} = \exp\left\{-\frac{m\omega}{\hbar}(x - a\cos\omega T)^2\right\}$$

[6] This solution is from team SciTech.

Probability amplitude at time T is a Gaussian function as it was at time $t = 0$. Normalizing this function we can reach the final result,

$$\int_{-\infty}^{\infty} |\psi(x,T)|^2 dx = \int_{-\infty}^{\infty} \exp\left\{-\frac{m\omega}{\hbar}(x - a\cos\omega T)^2\right\} dx = \sqrt{\frac{\pi\hbar}{m\omega}}$$

$$\Longrightarrow |\psi(x,T)|^2_{\text{normalized}} = \sqrt{\frac{m\omega}{\pi\hbar}} \exp\left\{-\frac{m\omega}{\hbar}(x - a\cos\omega T)^2\right\}$$

5.4 Exercise (4 pts)

Show that for arbitrary $f(t)$ resulting kernel is

$$K = \left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2} \exp\left\{\frac{iS_{\text{cl}}}{\hbar}\right\} \tag{60}$$

Answer: [7] We have shown in exercise 5.2 that

$$K(b,a) = F(T)\exp\left\{\frac{i}{\hbar}S_{cl}\right\} \tag{S17}$$

Since

$$\lim_{T\to 0} K(x_N, t_N; x_0, t_0) = \delta(x_N - x_0)$$

Integrating over dx_N gives

$$\lim_{T\to 0} F(T) \int dx_N \exp\left[\frac{i}{\hbar}S_{cl}\right] = 1.$$

In the classical action eq. 55, we see that as $T \to 0$, or $t_N \to t_0$, all the integrals involving f become significantly smaller than the other terms. Furthermore, the cosine term approaches 1. Thus we can approximate the action as

$$S_{cl} \approx \frac{m\omega}{2\sin(\omega T)}\left[x_N^2 + x_0^2 - 2x_N x_0\right]$$

in the small T limit. Doing the Gaussian integration gives

$$\left(\frac{2\pi i\hbar\sin(\omega T)}{m\omega}\right)^{1/2} F(T) = 1$$

Or

$$F(T) = \left(\frac{m\omega}{2\pi i\hbar\sin(\omega T)}\right)^{1/2}.$$

Therefore the desired propagator for the forced harmonic oscillator is

$$K = \left(\frac{m\omega}{2\pi i\hbar\sin(\omega T)}\right)^{1/2} \exp\left[\frac{i}{\hbar}S_{cl}\right]$$

[7] This solution is modified from team AceD's.

6 Partition Function

The partition function provides the link between microscopic properties of atoms and molecules and thermodynamic properties of matter. The latter one reflects the average behavior of many particles. In fact, the partition function provides a way to determine the most likely average behavior of atoms and molecules given information about the microscopic properties of the material.
Let us derive the partition function. Consider a system composed of N molecules. Although the system has a constant total energy of E, the energy may be distributed among the molecules in any number of ways. As molecules interact, the energy is continually redistributed between molecules and can switch between the various modes of motion. Instead of attempting to determine the energy of each individual molecule at every instant in time, we focus on the population of each energetic state. We would like to determine on average how many molecules, n_i, are in a particular energetic state, E_i. Over time the population of each state remains almost constant, although the individual molecules in each state may change at every collision. We also assume the ergodic hypothesis. This means that we assume *all states corresponding to a given energy are equally probable.*
There can be numerous different configurations of the system. Some possibilities include $\{N, 0, 0, ...\}$ with all of the molecules in the ground state E_0, or $\{N-1, 1, 0, ...\}$, where one of the molecules is in the excited state E_1 and all other particles are in the ground state. Of these two configurations, the second is much more likely, since any of the N molecules could be in the excited state resulting in a total of N possible arrangements of molecules. On the other hand there is only one possible way to get the first configuration, since all of the molecules must be in the ground state.

6.1 Exercise (2 pts)

Let W be the number of arrangements corresponding to a given configuration $\{n_0, n_1, ...\}$. Show that in the limit of large N,

$$\ln W = N \ln N - \sum(n_i \ln n_i) \tag{61}$$

Hint: use Stirling's approximation.
Answer: From combinatorics the number of arrangements can be written as

$$W = \frac{N!}{n_0! n_1! n_2! ...} \tag{S18}$$

When working with large numbers it is often convenient to work with ln(W) instead of W itself. For this case:

$$\begin{aligned} \ln W &= \ln \tfrac{N!}{n_0! n_1! n_2! ...} \\ &= \ln N! - \ln(n_0! n_1! n_2! ...) \qquad \text{(S19)} \\ &= \ln N! - \textstyle\sum_{i=0}^{m} \ln n_i! \qquad (2) \end{aligned}$$

Applying Stirling's approximation,

$$\ln n! \approx n \ln n - n \tag{S20}$$

and the fact that

$$N = \sum n_i \tag{S21}$$

gives

$$\begin{aligned} \ln W &= N \ln N - N - \sum(n_i \ln n_i - n_i) \\ &= N \ln N - \sum(n_i \ln n_i) \end{aligned} \tag{S22}$$

It was mentioned that the configuration {N-1,1,0...} dominates {N,0,0,...} because there are more ways to obtain it. We would expect there to be other configurations that dominate both of these. In fact we would expect the configuration with the largest value of W to dominate all other configurations.

6.2 Exercise (4 pts)

Show that in the most probable configuration, the number of particles with energy E_i is

$$n_i = \frac{N \exp(-\beta E_i)}{\sum_j \exp(-\beta E_j)} \tag{62}$$

Hint: You will need to use the method of Lagrange multipliers. To maximize some function $f(x) = g(x)$ subject to several constraints like

$$h_i(x) = 0 \tag{63}$$

You add these constraints to the objective function $f(x, \alpha_i)$ by

$$f(x, \alpha_i) = g(x) + \sum_i \alpha_i h_i(x) \tag{64}$$

Next step is to differentiate $f(x, \alpha_i)$ with respect to x and α_i

$$\frac{\partial f(x)}{\partial x} = 0, \quad h_i(x) = 0 \tag{65}$$

Solving this system of equations will give you the result. **Answer:** One way to find the maximum of ln(W) is to solve the equation:

$$\frac{\partial \ln(W)}{\partial n_i} = 0 \tag{S23}$$

However, Equation (S18) applies to the situation in which any arbitrary configuration n0, n1,... is possible. In reality there are a few constraints on the system that must be accounted for. First, since the total number of molecules is fixed at N, not all values of ni can be arbitrary. Instead only configurations in which:

$$N = \sum n_i \tag{S24}$$

are possible. Also, the total energy of the system is fixed at E. Therefore, since the total energy is the sum of the energies of all the individual molecules:

$$E = \sum n_i E_i \tag{S25}$$

We can find the maximum of ln(W) subject to the constraints on N and E expressed in equations (5) and (6) using the method of Lagrange multipliers as follows. First, we must rearrange the constraint equations as:

$$N - \sum n_i = 0 \quad \text{and} \quad E - \sum n_i E_i = 0 \tag{S26}$$

Next, we create a new function by multiplying the constraints by the arbitrary constants $-\alpha'$ and β, and adding them to the original function, ln(W), to get:

$$\begin{aligned} f(n_i) &= \ln(W) - \alpha' (N - \textstyle\sum n_i) + \beta (E - \textstyle\sum n_i E_i) \\ &= N \ln N - \textstyle\sum n_i \ln n_i - \alpha' (N - \textstyle\sum n_i) + \beta (E - \textstyle\sum n_i E_i) \end{aligned} \tag{S27}$$

Taking the derivative of Equation (S22) and setting the result to zero gives:

$$\frac{\partial f(n_i)}{\partial n_i} = -\left(1 + \ln(n_i)\right) + \alpha' - \beta E_i = 0 \tag{S28}$$

We define a new parameter $\alpha = \alpha' - 1$, giving:

$$-\ln(n_i) + \alpha - \beta E_i = 0 \tag{S29}$$

Solving this for ni gives the most probable population of state Ei:

$$n_i = \exp(\alpha - \beta E_i) \tag{S30}$$

Finally, we must evaluate the constants α and β. Substituting Equation (S25) back into Equation (S19) and solving for $\exp(\alpha)$ gives:

$$N = \sum n_i = \exp(\alpha) \sum \exp(-\beta E_i) \tag{S31}$$

$$\exp(\alpha) = \frac{N}{\sum \exp(-\beta E_i)} \tag{S32}$$

Changing the subscript to j and substituting this result back into Equation (S25) gives the Maxwell-Boltzmann distribution:

$$n_i = \frac{N \exp(-\beta E_i)}{\sum \exp(-\beta E_j)} \tag{S33}$$

The resultant equation follows the Boltzmann distribution. The term in the denominator is called the partition function and is defined as follows:

$$Z = \sum_j \exp\left(-\beta E_j\right) \tag{66}$$

As you see, the partition function provides a measure of the total number of energetic states that are accessible at a particular temperature and can be related to many different thermodynamic properties. We can define the probability of occurrence of some state i with energy E_i as

$$P_i = \frac{\exp(-\beta E_i)}{Z} \tag{67}$$

Now we can relate the thermodynamic properties of matter using partition function.

6.3 Exercise (3 pts)

Show that the average energy is expressed as

$$\overline{E} = -\frac{\partial \ln(Z)}{\partial \beta} \tag{68}$$

Answer: The mean energy is written

$$\bar{E} = \frac{\sum_r \exp\left(-\beta E_r\right) E_r}{\sum_r \exp\left(-\beta E_r\right)} \tag{S34}$$

where the sum is taken over all states of the system, irrespective of their energy. Note that

$$\sum_r \exp\left(-\beta E_r\right) E_r = -\sum_r \frac{\partial}{\partial \beta} \exp\left(-\beta E_r\right) = -\frac{\partial Z}{\partial \beta} \tag{S35}$$

where

$$Z = \sum_j \exp\left(-\beta E_j\right) \tag{S36}$$

It follows that

$$\overline{E} = -\frac{\partial \ln(Z)}{\partial \beta} \tag{S37}$$

6.4 Exercise (3 pts)

Show that the variance of energy is expressed as

$$\overline{(\Delta E)^2} = \frac{\partial^2 \ln(Z)}{\partial \beta^2} \tag{69}$$

Hint: use the expression

$$\sum_r \exp(-\beta E_r) E_r^2 = \left(\frac{-\partial}{\partial \beta}\right)^2 \left[\sum_r \exp(-\beta E_r)\right] \tag{70}$$

Answer: We can evaluate mean from

$$\overline{(\Delta E)^2} = \overline{E^2} - \bar{E}^2 \tag{S38}$$

according to the canonical distribution

$$\overline{E^2} = \frac{\sum_r \exp\left(-\beta E_r\right) E_r^2}{\sum_r \exp\left(-\beta E_r\right)} \tag{S39}$$

and we know that

$$\sum_r \exp\left(-\beta E_r\right) E_r^2 = -\frac{\partial}{\partial \beta}\left[\sum_r \exp\left(-\beta E_r\right) E_r\right] = \left(-\frac{\partial}{\partial \beta}\right)^2 \left[\sum_r \exp\left(-\beta E_r\right)\right]. \tag{S40}$$

Hence

$$\overline{E^2} = \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} \tag{S41}$$

Or we can write it as

$$\overline{E^2} = \frac{\partial}{\partial \beta}\left(\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right) + \frac{1}{Z^2}\left(\frac{\partial Z}{\partial \beta}\right)^2 = -\frac{\partial \bar{E}}{\partial \beta} + \bar{E}^2 \tag{S42}$$

and get

$$\overline{(\Delta E)^2} = -\frac{\partial \bar{E}}{\partial \beta} = \frac{\partial^2 \ln Z}{\partial \beta^2} \tag{S43}$$

Suppose that the system is characterized by a single external parameter x (for example volume). Consider a quasi-static change of the external parameter from x to $x + dx$.

6.5 Exercise (4 pts)

Find the macroscopic work done by system dW. (Hint: you can use the fact that small increment of function $y = f(x)$ can be related as $\delta y = \frac{df(x)}{dx}\delta x$)

Answer:

In this process, the energy of the system in state r changes by

$$\delta E_r = \frac{\partial E_r}{\partial x} dx \tag{S44}$$

The macroscopic work $đW$ done by the system due to this parameter change is

$$\vec{a} = \frac{\sum_r \exp\left(-\beta E_r\right)\left(-\partial E_r/\partial x dx\right)}{\sum_r \exp\left(-\beta E_r\right)} \tag{S45}$$

In other words, the work done is minus the average change in internal energy of the system, where the average is calculated using the canonical distribution. We can write

$$\sum_r \exp\left(-\beta E_r\right)\frac{\partial E_r}{\partial x} = -\frac{1}{\beta}\frac{\partial}{\partial x}\left[\sum_r \exp\left(-\beta E_r\right)\right] = -\frac{1}{\beta}\frac{\partial Z}{\partial x}, \tag{S46}$$

which gives

$$dW = \frac{1}{\beta Z}\frac{\partial Z}{\partial x}dx = \frac{1}{\beta}\frac{\partial \ln Z}{\partial x}dx \tag{S47}$$

6.6 Exercise (4 pts)

Suppose that $x = V$. Using the expression of work in the last exercise, show that average pressure can be represented as

$$\overline{p} = \frac{1}{\beta}\frac{\partial \ln(Z)}{\partial V} \tag{71}$$

Answer: The general equation of work is

$$dW = pdV \tag{S48}$$

Comparing it with the previous result given the $x = V$ we get

$$\overline{p} = \frac{1}{\beta}\frac{\partial \ln(Z)}{\partial V} \tag{S49}$$

Because the partition function is a function of β and V (the energies E_r depend on V), it follows that the previous equation relates the mean pressure, $\overline{p}$, to T (via $\beta = 1/kT$) and V .

All important macroscopic quantities associated with a system can be expressed in terms of its partition function Z. Let us investigate how the partition function is related to thermodynamic quantities. Recall that Z is a function of both β and x. Hence, $Z = Z(x, \beta)$.

6.7 Exercise (4 pts)

Consider a quasi-static change by which x and β change so slowly that the system stays close to equilibrium, and, thus, remains distributed according to the Boltzmann distribution. Find the expression of entropy of a system from its partition function. (Hint: You can use the first law of thermodynamics and equation $dS = \frac{dQ}{T}$)

Answer: Because partition function depends on two parameters we can write

$$d \ln Z = \frac{\partial \ln Z}{\partial x} dx + \frac{\partial \ln Z}{\partial \beta} d\beta \tag{S50}$$

Using the previous results of mean energy and work

$$d \ln Z = \beta dW - \bar{E} d\beta = \beta dW - d(\bar{E}\beta) + \bar{E} d\beta \tag{S51}$$

giving

$$d(\ln Z + \beta \bar{E}) = \beta(\vec{d}W + d\bar{E}) \equiv \beta dQ \tag{S52}$$

Using the second law of thermodynamics we get

$$S = k(\ln Z + \beta \bar{E}) \tag{S53}$$

6.8 Exercise (2 pts)

Suppose we are dealing with system that consists of two subsystem. By using the partition function, prove that the extensive thermodynamic functions (Energy and Entropy) of two weakly-interacting systems are simply additive.

Answer: Suppose that we are dealing with a system $A^{(0)}$ consisting of two systems A and A' that only interact weakly with one another. Let each state of A be denoted by an index r , and have a corresponding energy E_r . Likewise, let each state of A' be denoted by an index s , and have a corresponding energy E'_s . A state of the combined system $A^{(0)}$ is then denoted by two indices r and s . Because A and A' only interact weakly, their energies are additive, and the energy of state rs is

$$E^{(0)}_{rs} = E_r + E'_s \tag{S54}$$

By definition, the partition function of $A^{(0)}$ takes the form

$$\begin{aligned} Z^{(0)} &= \sum_{r,s} \exp\left[-\beta E^{(0)}_{rs}\right] = \sum_{r,s} \exp\left(-\beta\left[E_r + E'_s\right]\right) = \sum_{r,s} \exp\left(-\beta E_r\right) \exp\left(-\beta E'_s\right) \\ &= \left[\sum_r \exp\left(-\beta E_r\right)\right] \left[\sum_s \exp\left(-\beta E'_s\right)\right]. \end{aligned} \tag{S55}$$

hence

$$Z^{(0)} = Z Z' \tag{S56}$$

giving

$$\ln Z^{(0)} = \ln Z + \ln Z' \tag{S57}$$

From previous equations we get mean energy and entropy as

$$\bar{E}^{(0)} = \bar{E} + \bar{E}' \tag{S58}$$

$$S^{(0)} = S + S' \tag{S59}$$

7 Path Integral Calculation of Partition Function

Let $\{|j\rangle\}$ be a set of energy eigenstates, then the partition function is[8]

$$Z = \sum_j \left\langle j \left| e^{-\beta H} \right| j \right\rangle \tag{72}$$

There is a connection between this formula and the propagator eq. 46:

7.1 Exercise (3 pts)

Let $t - t_0 = -i\beta\hbar$, show that

$$Z = \int dx\, U\left(x, -i\beta\hbar; x, 0\right) \tag{73}$$

Answer:

$$\begin{aligned}
Z &= \sum_j \int dx \int dy \left\langle j \left| x \right\rangle \langle x | e^{-\beta H} | y \rangle \langle y \right| j \right\rangle \\
&= \sum_j \int dx \int dy \langle y | j \rangle \left\langle j \left| x \right\rangle \langle x | e^{-\beta H} | y \rangle \right. \\
&= \int dx \int dy \langle y | x \rangle \langle x | e^{-\beta H} | y \rangle \\
&= \int dy \langle y | e^{-\beta H} | y \rangle \\
&= \int dx\, U\left(x, -i\beta\hbar; x, 0\right)
\end{aligned}$$

where

$$U\left(x, t; x, 0\right) = \left\langle x \left| e^{-i\hat{H}t/\hbar} \right| x \right\rangle \tag{S60}$$

7.2 Exercise (5 pts)

Use eq. 73 to calculate the partition function of quantum harmonic oscillator at inverse temperature β.

[8] I have omitted the "hat" symbol over the Hamiltonian operator $\hat{H}$ for the rest of the competition. So $H = \hat{H}$ is the Hamiltonian operator. I hope this does not cause any confusion.

Answer: Using eq. 56,

$$
\begin{aligned}
Z &= \int dx\; U\left(x, -i\beta\hbar; x, 0\right) \\
&= \int dx \left(\frac{m\omega}{2\pi\hbar i \sin(-i\beta\hbar\omega)}\right)^{1/2} \exp\left\{\frac{-m\omega}{\hbar i \sin(-i\beta\hbar\omega)}\left[x^2\cos(-i\beta\hbar\omega) - x^2\right]\right\} \\
&= \left(\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right)^{1/2} \int dx \exp\left\{\frac{-m\omega x^2}{\hbar\sinh(\beta\hbar\omega)}[\cosh(\beta\hbar\omega) - 1]\right\} \\
&= \left(\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right)^{1/2} \left(\frac{\pi}{\frac{m\omega}{\hbar\sinh(\beta\hbar\omega)}[\cosh(\beta\hbar\omega) - 1]}\right)^{1/2} \\
&= [2(\cosh(\beta\hbar\omega) - 1)]^{-1/2}
\end{aligned}
$$

7.3 Exercise (3 pts)

More generally, let $t = -i\tau$, show that the propagator becomes

$$
U\left(x_1, -i\tau; x_0\right) = \int Dx\; \exp\left[-\frac{1}{\hbar} S_E[x(\tau)]\right] \tag{74}
$$

where the *Euclidean action* is $S_E[x(\tau)] = \int_{x(\tau_1)=x_0}^{x(\tau_2)=x_1} d\tau \left(\frac{m}{2}\dot{x}^2(\tau) + V(x(\tau))\right)$. Note that the sign of the potential energy is inverted.
Answer:

$$
\begin{aligned}
U\left(x_1, -i\tau; x_0, 0\right) &= \int_{x(0)=x_0}^{x(-i\tau)=x_1} \mathcal{D}x\; \exp\left[\frac{i}{\hbar}\int_0^{-i\tau} dt\mathcal{L}\right] \\
&= \int \mathcal{D}x\; \exp\left[\frac{1}{\hbar}\int_0^{\tau} d\tau' \left(\frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x)\right)\right] \\
&= \int \mathcal{D}x\; \exp\left[\frac{-1}{\hbar}\int_0^{\tau} d\tau' \left(\frac{m}{2}\left(\frac{dx}{d\tau'}\right)^2 + V(x(\tau))\right)\right]
\end{aligned}
$$

This process is called *Wick rotation*. For a theory with inverse temperature β, section 7.1 shows that the partition function can be calculated by path integral on an Euclidean τ circle of length β.

8 Green's Function in Quantum Mechanics

We will develop a path integral representation of n-point correlation function in quantum mechanics:

$$G^{(n)}(t_1, t_2, \cdots, t_n) = \langle \Omega | T\hat{x}(t_1)\hat{x}(t_2)\cdots\hat{x}(t_n) | \Omega \rangle \tag{75}$$

where $|\Omega\rangle$ is the ground state of the system and $\hat{x}(t) = e^{i\hat{H}t}\hat{x}e^{-i\hat{H}t}$ is the Heisenberg picture operator at time t.[9]. In the next section we will use these correlation functions to calculate scattering amplitudes based on Feynman diagrams.
When $n = 2$, the 2-point correlation function becomes the standard time-ordered Green's function. The *time-ordered operator* T is defined as:

$$T\hat{x}(t_1)\hat{x}(t_2) = \begin{cases} \hat{x}(t_1)\hat{x}(t_2) & t_1 > t_2 \\ \hat{x}(t_2)\hat{x}(t_1) & t_2 > t_1 \end{cases} \tag{76}$$

where the earliest operator is written last (right-most), the second earliest second last, etc.
Consider

$$\int \mathcal{D}x\ x(t_1)x(t_2)\exp\left[i\int_{-T}^{T} dt\ \mathcal{L}(t)\right] \tag{77}$$

where **the boundary conditions are** $x(-T) = x_a$ **and** $x(T) = x_b$[10]. Break up the functional integral into three parts:

$$\int \mathcal{D}x = \int dx_1 \int dx_2 \quad \int_{x(t_1)=x_1, x(t_2)=x_2} \quad \mathcal{D}x \tag{78}$$

8.1 Exercise (4 pts)

Show that when $t_1 < t_2$, eq. 77 is equal to

$$\left\langle x_b \left| e^{-iH(T-t_2)}\hat{x}\ e^{-iH(t_2-t_1)}\hat{x}\ e^{-iH(t_1+T)} \right| x_a \right\rangle \tag{79}$$

where $\hat{x}$ is position operator that satisfies $\hat{x}|x_0\rangle = x_0|x_0\rangle$. Consequently show that eq. 77 is equal to

$$\left\langle x_b \left| e^{-iHT}\ \mathrm{T}\{\hat{x}(t_1)\hat{x}(t_2)\}\ e^{-iHT} \right| x_a \right\rangle \tag{80}$$

[9]Just think of it as the definition of operator at time t. The Heisenberg picture is another equivalent description where the wave function doesn't change with time but the operator evolves in time. You can read more about it on Wikipedia's page on Heisenberg picture, but the details are not important here.

[10]For simplicity, we will set $\hbar = 1$ for the rest of this competition (this is called natural units). This can significantly simplify notation. You can use dimensional analysis to add appropriate powers of $\hbar$ to convert back to SI units.

Answer: When $t_1 < t_2$,

$$\begin{aligned}
&\int \mathcal{D}x\ x(t_1)x(t_2) \exp\left[i\int_{-T}^{T} dt\ \mathcal{L}(t)\right] \\
&= \int dx_1 \int dx_2 \quad \int_{x(t_1)=x_1, x(t_2)=x_2} \mathcal{D}x\ x_1x_2 \exp\left[i\int_{-T}^{T} dt\ \mathcal{L}(t)\right]
\end{aligned} \tag{S61}$$

We also have the boundary conditions $x(-T) = x_a$ and $x(T) = x_b$. Using eq. 46 for the intervals $(-T, t_1), (t_1, t_2), (t_2, T)$, we have

$$\begin{aligned}
&\int_{x(t_1)=x_1, x(t_2)=x_2} \mathcal{D}x\ \exp\left[i\int_{-T}^{T} dt\ \mathcal{L}(t)\right] \\
&= \left\langle x_b \left| e^{-iH(T-t_2)} |x_2\rangle\langle x_2| e^{-iH(t_2-t_1)} |x_1\rangle\langle x_1|\ e^{-iH(t_1+T)} \right| x_a \right\rangle
\end{aligned} \tag{S62}$$

Therefore

$$\begin{aligned}
&\int \mathcal{D}x\ x(t_1)x(t_2) \exp\left[i\int_{-T}^{T} dt\ \mathcal{L}(t)\right] \\
&= \int dx_1 \int dx_2 \left\langle x_b \left| e^{-iH(T-t_2)} x_2 |x_2\rangle\langle x_2| e^{-iH(t_2-t_1)} x_1 |x_1\rangle\langle x_1|\ e^{-iH(t_1+T)} \right| x_a \right\rangle \\
&= \int dx_1 \int dx_2 \left\langle x_b \left| e^{-iH(T-t_2)} \hat{x} |x_2\rangle\langle x_2| e^{-iH(t_2-t_1)} \hat{x} |x_1\rangle\langle x_1|\ e^{-iH(t_1+T)} \right| x_a \right\rangle \\
&= \left\langle x_b \left| e^{-iH(T-t_2)} \hat{x}\ e^{-iH(t_2-t_1)} \hat{x}\ e^{-iH(t_1+T)} \right| x_a \right\rangle \\
&= \left\langle x_b \left| e^{-iHT} \hat{x}(t_2)\hat{x}(t_1)\ e^{-iHT} \right| x_a \right\rangle
\end{aligned} \tag{S63}$$

When $t_1 > t_2$, we need to interchange t_1, t_2 in all the expressions above, so together we have the time-ordered product $\mathrm{T}\{\hat{x}(t_1)\hat{x}(t_2)\}$.

8.2 Exercise (4 pts)

Prove

$$G(t_1, t_2) = \lim_{T\to\infty(1-i\epsilon)} \frac{\int \mathcal{D}x\ x(t_1)\, x(t_2)\, e^{i\int_{-T}^{T} dt\ \mathcal{L}(t)}}{\int \mathcal{D}x\ e^{i\int_{-T}^{T} dt\ \mathcal{L}(t)}} \tag{81}$$

where $\epsilon > 0$ is a *small* positive number. (Hint: First prove

$$e^{-iHT} |x_a\rangle \underset{T\to\infty(1-i\epsilon)}{\longrightarrow} \langle \Omega \mid x_a\rangle\, e^{-iE_0\cdot\infty(1-i\epsilon)} |\Omega\rangle \tag{82}$$

where $|\Omega\rangle$ is the ground state.)

Answer: Let the energy eigenstates be $|n\rangle$. Assume the state $|x_a\rangle$ has nonzero overlap with the ground state, so $\langle \Omega \mid x_a\rangle \neq 0$ (which is nearly always the case in practice).

$$e^{-iHT}|x_a\rangle = \sum_n e^{-iE_nT}|n\rangle\langle n \mid x_a\rangle = \sum_n e^{-iE_0T}e^{-i(E_n-E_0)T}|n\rangle\langle n \mid x_a\rangle$$
$$\xrightarrow[T\to\infty(1-i\epsilon)]{} \langle\Omega \mid x_a\rangle\, e^{-iE_0\cdot\infty(1-i\epsilon)}|\Omega\rangle$$

because all the other states are exponentially suppressed by $\lim_{t\to\infty} e^{-(E_n-E_0)t\epsilon}$.

$$\begin{aligned}&\lim_{T\to\infty(1-i\epsilon)}\int \mathcal{D}x\; x(t_1)x(t_2)\exp\left[i\int_{-T}^{T} dt\;\mathcal{L}(t)\right]\\ &=\langle x_b \mid \Omega\rangle\, e^{-iE_0\cdot\infty(1-i\epsilon)}\langle\Omega|\,\mathrm{T}\{\hat{x}(t_1)\hat{x}(t_2)\}\,|\Omega\rangle e^{-iE_0\cdot\infty(1-i\epsilon)}\langle\Omega \mid x_a\rangle\end{aligned} \tag{S64}$$

On the other hand,

$$\int \mathcal{D}x\; e^{i\int_{-T}^{T} dt\;\mathcal{L}(t)} = \langle x_b\left|e^{-i\hat{H}2T}\right|x_a\rangle \tag{S65}$$

So by dividing these two formulas we can get rid of the unwanted factors and get the desired result.

Generally we have

$$G^{(n)}\left(t_1, t_2, \cdots, t_n\right) = \lim_{T\to\infty(1-i\epsilon)} \frac{\int \mathcal{D}x\; x\left(t_1\right)x\left(t_2\right)\cdots x\left(t_n\right)e^{i\int_{-T}^{T} dt\;\mathcal{L}(t)}}{\int \mathcal{D}x\; e^{i\int_{-T}^{T} dt\;\mathcal{L}(t)}} \tag{83}$$

This expression is still too complicated. We will now give a smart way of reducing n-point functions to products of 2-point functions. Define the *generating functional*:

$$Z[J] = \frac{\int \mathcal{D}x\; e^{i(S+\int dt J(t)x(t))}}{\int \mathcal{D}x\; e^{iS}} \tag{84}$$

8.3 Exercise (4 pts)

Prove

$$\left.\left(\frac{1}{i}\frac{\delta}{\delta J\left(t_1\right)}\cdots\frac{1}{i}\frac{\delta}{\delta J\left(t_n\right)}Z[J]\right)\right|_{J=0} = \langle\Omega\left|T\hat{x}\left(t_1\right)\cdots\hat{x}\left(t_n\right)\right|\Omega\rangle \tag{85}$$

Answer: This is immediate from the definition of functional derivative below (the exponential function is defined using Taylor series):

$$\left(\frac{1}{i}\frac{\delta}{\delta J\left(t_{1}\right)}\cdots\frac{1}{i}\frac{\delta}{\delta J\left(t_{n}\right)}Z[J]\right)=\frac{\int\mathcal{D}x\ x(t_{1})\cdots x(t_{n})e^{i(S+\int dtJ(t)x(t))}}{\int\mathcal{D}x\ e^{iS}} \tag{S66}$$

By taking $J=0$ we get the desired result. We have assumed that the action S is computed in $T\to\infty(1-i\epsilon)$ limit, which is always to be assumed for the rest of this competition unless otherwise stated.

For the rest of this section, our Lagrangian is the harmonic oscillator Lagrangian $L_0=\frac{1}{2}(\partial_t x)^2-\frac{\omega^2}{2}x^2$. We have re-scaled x to absorb the m factor, because for harmonic oscillator only the ratio $\omega^2=k/m$ matters. We will prove that

$$Z[J]=\exp\left[-\frac{1}{2}\int dtdt'J(t)G\left(t,t'\right)J\left(t'\right)\right] \tag{86}$$

The proof is constructed in several steps:

8.4 Exercise (4 pts)

(Equation of motion for Green's function) A change of variable does not alter the functional intergral:

$$\int\mathcal{D}x\ x\left(t_{1}\right)e^{i\int_{-T}^{T}dt\ \mathcal{L}[x]}=\int\mathcal{D}x\ x'\left(t_{1}\right)e^{i\int_{-T}^{T}dt\ \mathcal{L}[x']} \tag{87}$$

for $x'(t)=x(t)+\epsilon(t)$ s.t. $\epsilon(-T)=\epsilon(T)=0$. $Dx=Dx'$.

Consider the harmonic oscillator Lagrangian $L_0=\frac{1}{2}(\partial_t x)^2-\frac{\omega^2}{2}x^2$. Expand this equation to first order in ϵ to show that

$$\int\mathcal{D}x\ e^{i\int_{-T}^{T}dt\ \mathcal{L}_0[x]}\int_{-T}^{T}dt\ \epsilon(t)\left((\partial_t^2+\omega^2)x(t)x(t_1)+i\delta(t-t_1)\right)=0 \tag{88}$$

And consequently conclude that

$$\left(\partial_t^2+\omega^2\right)\langle 0\left|T\hat{x}(t)\hat{x}(t_1)\right|0\rangle=-i\delta\left(t-t_1\right) \tag{89}$$

Answer: Eq. 87 implies

$$\int\mathcal{D}x\ \left[\epsilon\left(t_{1}\right)e^{i\int_{-T}^{T}dt\ \mathcal{L}[x]}+x(t_1)\left(i\int_{-T}^{T}dt\ \delta\mathcal{L}_0[x]\right)e^{i\int_{-T}^{T}dt\ \mathcal{L}_0[x]}\right]=0 \tag{S67}$$

$$\int_{-T}^{T}dt\ \delta\left(\frac{1}{2}(\partial_t x)^2\right)=-\int_{-T}^{T}dt\ \partial_t^2 x\delta x(t)=-\int_{-T}^{T}dt\ \partial_t^2 x\ \epsilon(t) \tag{S68}$$

where we have used partial integration and the boundary term is zero because $\epsilon(-T)=\epsilon(T)=0$.

$$\int_{-T}^{T}dt\ \delta\mathcal{L}_0[x]=-\int_{-T}^{T}dt\ \epsilon(t)(\partial_t^2+\omega^2)x(t) \tag{S69}$$

Putting everything together we get

$$\int \mathcal{D}x \; e^{i\int_{-T}^{T} dt \; \mathcal{L}_0[x]} \int_{-T}^{T} dt \; \epsilon(t) \left((\partial_t^2 + \omega^2)x(t)x(t_1) + i\delta(t - t_1)\right) = 0 \tag{S70}$$

Take $\epsilon(t) = \delta(t_0)$ so that we can restrict the equation to a particular time t_0:

$$\int \mathcal{D}x \; e^{i\int_{-T}^{T} dt \; \mathcal{L}_0[x]} \left((\partial_{t_0}^2 + \omega^2)x(t_0)x(t_1) + i\delta(t_0 - t_1)\right) = 0 \tag{S71}$$

Dividing by $\int \mathcal{D}x \; e^{i\int_{-T}^{T} dt \; \mathcal{L}_0[x]}$ and taking $T \to \infty(1 - i\epsilon)$ limit we get

$$\left(\partial_t^2 + \omega^2\right) \langle 0 \left| T\hat{x}(t)\hat{x}(t_1) \right| 0 \rangle = -i\delta\left(t - t_1\right) \tag{S72}$$

Note: Many of you wrote

$$\left(\partial_t^2 + \omega^2\right) x(t)x(t_1) = -i\delta\left(t - t_1\right) \tag{S73}$$

somewhere in your answer. Though I did not deduct points for this, this is *wrong*: for an arbitrary path there is no way the equation would hold. Instead, you need to keep the path integral $\int \mathcal{D}x \; e^{i\int_{-T}^{T} dt \; \mathcal{L}_0[x]}$, and after summing over all possible paths the equation holds.

We define *functional derivative* as follow:

$$\frac{\delta}{\delta J(x)} J(y) = \delta(x - y) \quad \text{or} \quad \frac{\delta}{\delta J(x)} \int dy \; J(y)\phi(y) = \phi(x) \tag{90}$$

It is a natural generalization of the following identities for discrete vectors:

$$\frac{\partial}{\partial x_i} x_j = \delta_{ij} \quad \text{or} \quad \frac{\partial}{\partial x_i} \sum_j x_j k_j = k_i \tag{91}$$

8.5 Exercise (4 pts)

Under a shift of the field:

$$x'(t) \equiv x(t) - i\int dt' \; G(t, t')J(t') \tag{92}$$

Prove that

$$\int dt \; (\mathcal{L}_0[x] + Jx) = \int dt \frac{1}{2}\left[x'\left(-\partial^2 - \omega^2\right)x'\right] - \frac{1}{2}\int dtdt' J(t)(-i)G\left(t, t'\right)J\left(t'\right) \tag{93}$$

and

$$Z[J] = \exp\left[-\frac{1}{2}\int dtdt' J(t)G\left(t, t'\right)J\left(t'\right)\right] \tag{94}$$

Answer: First note that by partial integration we have

$$\int dt\ \mathcal{L}_0[x] = \int dt \frac{1}{2} x \left(-\partial^2 - \omega^2\right) x \tag{S74}$$

So

$$\int dt \frac{1}{2}\left[x'\left(-\partial^2 - \omega^2\right) x'\right] - \frac{1}{2}\int dt dt' J(t)(-i) G\left(t, t'\right) J\left(t'\right)$$
$$= \int dt\ \left[\mathcal{L}_0[x] - \int dt'\ G(t,t')J(t')\frac{1}{2}\left(-\partial_t^2 - \omega^2\right)\int dt''\ G(t,t'')J(t'')\right.$$
$$\left. -\frac{i}{2}x(t)\left(-\partial^2 - \omega^2\right)\int dt'\ G(t,t')J(t') - \frac{i}{2}\int dt'\ G(t,t')J(t')\left(-\partial^2 - \omega^2\right)x(t)\right]$$
$$-\frac{1}{2}\int dt dt' J(t)(-i) G\left(t, t'\right) J\left(t'\right)$$

Using eq. 89, $\left(-\partial_t^2 - \omega^2\right)\langle 0\,|T\hat{x}(t)\hat{x}(t_1)|\,0\rangle = i\delta\left(t - t_1\right)$, the second term and the last term cancel:

$$\text{RHS}$$
$$= \int dt\ \left[\mathcal{L}_0[x] - \int dt'\ G(t,t')J(t')\frac{i}{2}\int dt''\ \delta(t-t'')J(t'')\right.$$
$$\left. +\frac{1}{2}x(t)\int dt'\ \delta(t-t')J(t') + \frac{1}{2}\int dt'\ \delta(t-t')J(t')x(t)\right] \text{ (Partial integration twice)}$$
$$-\frac{1}{2}\int dt dt' J(t)(-i) G\left(t, t'\right) J\left(t'\right)$$
$$= \int dt\ \left(\mathcal{L}_0[x] + x(t)J(t)\right)$$

Finally recall the definition of Z,

$$\begin{aligned} Z[J] &= \frac{\int \mathcal{D}x\ e^{i(S + \int dt J(t) x(t))}}{\int \mathcal{D}x\ e^{iS}} \\ &= \frac{\int \mathcal{D}x\ e^{i\int dt \mathcal{L}_0[x'] - \frac{1}{2}\int dt dt' J(t) G\left(t,t'\right) J\left(t'\right)}}{\int \mathcal{D}x\ e^{iS}} \\ &= e^{-\frac{1}{2}\int dt dt' J(t) G\left(t,t'\right) J\left(t'\right)} \end{aligned}$$

where from second to third line we have used $\mathcal{D}x = \mathcal{D}x'$ since a shift of x does not change the measure.

Now we are ready to prove (one of) the most important theorems in physics: Wick's theorem.

8.6 Exercise (3 pts)

Use equation 85 to prove that the correlation function of odd number of operators vanish:

$$\langle \mathrm{T}\,\hat{x}\left(t_{2N+1}\right)\hat{x}\left(t_{2N}\right)\cdots\hat{x}(1)\rangle = 0 \tag{95}$$

Answer:

$$
\begin{aligned}
&\langle \Omega \left| T\hat{x}\left(t_1\right) \cdots \hat{x}\left(t_n\right) \right| \Omega \rangle \\
=&\left(\frac{1}{i}\frac{\delta}{\delta J\left(t_1\right)} \cdots \frac{1}{i}\frac{\delta}{\delta J\left(t_n\right)} \exp\left[-\frac{1}{2}\int dtdt' J(t)G\left(t,t'\right)J\left(t'\right)\right]\right)\Bigg|_{J=0}
\end{aligned}
$$

Since

$$
\begin{aligned}
&\frac{1}{i}\frac{\delta}{\delta J\left(t_1\right)} \exp\left[-\frac{1}{2}\int dtdt' J(t)G\left(t,t'\right)J\left(t'\right)\right] \\
=&i\int dt'\ G(t_1,t')J(t') \exp\left[-\frac{1}{2}\int dtdt' J(t)G\left(t,t'\right)J\left(t'\right)\right]
\end{aligned}
$$

Hence after n derivatives, the result is a polynomial in J times the exponential. Every time the derivative acts on the exponential, another J will appear; every time the derivative acts on the polynomial (in J) coefficient in the front, the order of every term in the polynomial will decrease by 1. So all the terms in the polynomial coefficient have either odd degree (n odd) or even degree (n even). When we take $J = 0$ in the end, the exponential will become 1 and only the constant term in the polynomial will survive. When n is odd, there is no constant term, so the n-point function is zero.

8.7 Exercise (4 pts)

For even number of operators we have

$$
\langle \mathrm{T}\,\hat{x}\left(t_{2N}\right)\hat{x}\left(t_{2N-1}\right)\cdots\hat{x}(1)\rangle = \sum_{i_k>j_k, i_{k+1}>i_k} \langle \hat{x}\left(t_{i_N}\right)\hat{x}\left(t_{j_N}\right)\rangle \cdots \langle \hat{x}\left(t_{i_1}\right)\hat{x}\left(t_{j_1}\right)\rangle \tag{96}
$$

The RHS looks very complicated, but it is just the sum over all possible pair of operators (see next equation for an example). The idea of the general proof is already present in a special case:

$$
\langle 0 \left| T\hat{x}_1\hat{x}_2\hat{x}_3\hat{x}_4 \right| 0\rangle = G_{34}G_{12} + G_{24}G_{13} + G_{14}G_{23} \tag{97}
$$

where $\hat{x}_i$ stands for $\hat{x}(t_i)$ and $G_{ij} = G(t_i, t_j)$. Prove this special case.

Answer: Just use eq. 85 and 94 for $n = 4$. A brute-force calculation can yield the desired result.

8.8 Exercise (6 pts)

For quantum harmonic oscillator, use eq. 85, 55, 60 to show that

$$
G(t_2, t_1) = \frac{1}{2\omega} e^{-i\omega|t_2-t_1|} \tag{98}
$$

Hint: write $\cos(x) = \frac{e^{ix}+e^{-ix}}{2}$ and $\sin(x) = \frac{e^{ix}-e^{-ix}}{2i}$. Take $x_a = x_b = 0$ to simplify your expressions.

Answer: The source $J(t)$ defined above is proportional to the force $f(t)$ in driven harmonic oscillator (you can apply Euler-Lagrange equation to $\mathcal{L} = \mathcal{L}_0[x] + Jx$ to see this). As we are going to take $J = 0$ in the end, it does not matter what the proportionality constant is, since we can always re-scale J or f to make them equal. Therefore, we can identify $f(t)$ to be $J(t)$. The propagator, or kernel, of a driven harmonic oscillator is (eq. 60):

$$K(x_b, t_b; x_a, t_a) = \left(\frac{m\omega}{2\pi i\hbar \sin\omega T'}\right)^{1/2} \exp\left\{\frac{iS_{\text{cl}}}{\hbar}\right\} \tag{S75}$$

where $T' = t_b - t_a$ and (eq. 55)

$$\begin{aligned} S_{\text{cl}} =& \frac{m\omega}{2\sin\omega T'}\left[\cos\omega T'\left(x_b^2 + x_a^2\right) - 2x_b x_a\right.\\ &+ \frac{2x_a}{m\omega}\int_{t_a}^{t_b} \sin(\omega\,(t_b - t)) f(t)\mathrm{d}t + \frac{2x_b}{m\omega}\int_{t_a}^{t_b} \sin(\omega\,(t - t_a)) f(t)\mathrm{d}t \\ &\left.- \frac{2}{m^2\omega^2}\int_{t_a}^{t_b}\int_{t_a}^{t} \sin(\omega\,(t_b - t))\sin(\omega\,(t' - t_a)) f\left(t'\right) f(t)\mathrm{d}t'\mathrm{d}t\right] \end{aligned} \tag{S76}$$

K is precisely the numerator of eq. 84 before taking $T \to \infty(1 - i\epsilon)$. So

$$\begin{aligned} Z = \exp&\left[\frac{i}{\hbar}\frac{m\omega}{2\sin\omega T'}\left[\frac{2x_a}{m\omega}\int_{t_a}^{t_b} \sin(\omega\,(t_b - t)) f(t)\mathrm{d}t + \frac{2x_b}{m\omega}\int_{t_a}^{t_b} \sin(\omega\,(t - t_a)) f(t)\mathrm{d}t\right.\right. \\ &\left.\left.- \frac{2}{m^2\omega^2}\int_{t_a}^{t_b}\int_{t_a}^{t} \sin(\omega\,(t_b - t))\sin(\omega\,(t' - t_a)) f\left(t'\right) f(t)\mathrm{d}t'\mathrm{d}t\right]\right] \end{aligned}$$

and $t_a = -T, t_b = T$. Note that $T' = t_b - t_a = 2T$, a slight confusion of notation between different sections. As G does not depend on initial or final state in the path integral (the limit $T \to (1 - i\epsilon)\infty$ projects onto the ground state only, as shown in eq. 82), we can safely choose $x_a = x_b = 0$ to simplify our calculations. We are left with:

$$Z = \exp\left[-\frac{i}{\hbar}\frac{1}{\sin\omega T'}\frac{1}{m\omega}\int_{t_a}^{t_b}\int_{t_a}^{t} \sin(\omega\,(t_b - t))\sin(\omega\,(t' - t_a)) f\left(t'\right) f(t)\mathrm{d}t'\mathrm{d}t\right] \tag{S77}$$

Consider the case when $t_1 < t_2$. After taking $f = 0$ below, only the term with two derivatives acting on the exponent survives. Since $t' \le t$ by the integration range of t', the functional derivatives will give $\delta(t' - t_1), \delta(t - t_2)$.

$$\left.\left(\frac{1}{i}\frac{\delta}{\delta f\left(t_1\right)}\frac{1}{i}\frac{\delta}{\delta f\left(t_2\right)} Z\right)\right|_{f=0} = \frac{i}{\hbar}\frac{1}{\sin\omega T'}\frac{1}{m\omega}\sin(\omega\,(t_b - t_2))\sin(\omega\,(t_1 - t_a)) \tag{S78}$$

Now it is time for some algebra:

$$\begin{aligned} &\sin(\omega\,(t_b - t_2))\sin(\omega\,(t_1 - t_a)) \\ =& \frac{1}{2}(\cos(\omega(t_a + t_b - t_1 - t_2)) - \cos(\omega(t_b - t_a + t_1 - t_2))) \\ =& \frac{1}{2}(\cos(\omega(t_1 + t_2)) - \cos(\omega(2T + t_1 - t_2))) \end{aligned}$$

Under $T \to (1 - i\epsilon)\infty$, $\sin(\omega T) \sim \frac{e^{i\omega T}}{2i}$ and $\cos(\omega T) \sim \frac{e^{i\omega T}}{2}$ because $-i\epsilon\infty$ term makes $|e^{i\omega T}| \to \infty$ and $e^{-i\omega T} \to 0$. Eq. S78 becomes

$$\begin{aligned}
&\frac{i}{2\hbar}\frac{2i}{e^{i\omega 2T}}\frac{1}{m\omega}\left(\cos(\omega(t_1+t_2)) - \frac{e^{i\omega(2T+t_1-t_2)}}{2}\right) \\
\sim&\frac{1}{2\hbar m\omega}\frac{e^{i\omega(2T+t_1-t_2)}}{e^{i\omega 2T}} \\
\sim&\frac{1}{2\hbar m\omega}e^{i\omega(t_1-t_2)}
\end{aligned}$$

Since we have set $m = 1$ in the definition of $\mathcal{L}_0$ and $\hbar = 1$ in natural unit,

$$G(t_2, t_1) = \frac{1}{2\omega}e^{-i\omega(t_2-t_1)} \tag{S79}$$

When $t_1 > t_2$, just exchange 1 and 2 in the proof above and we get

$$G(t_2, t_1) = \frac{1}{2\omega}e^{-i\omega|t_2-t_1|} \tag{S80}$$

9 Feynman Diagram

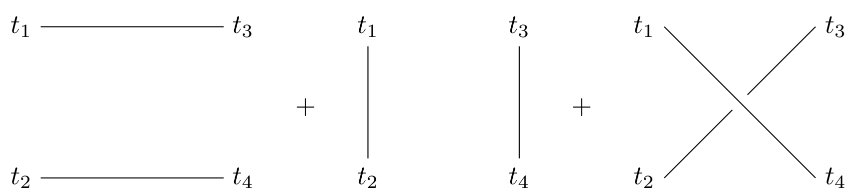
Now we add a small perturbation to the harmonic oscillator Lagrangian L_0: $\mathcal{L} = \mathcal{L}_0 - \frac{\lambda}{4!}x^4$. In this example the theory can still be analytically solved, but in general the theory becomes unsolvable (no analytic expression). We will assume $\lambda \ll 1$ and use Taylor expansion to compute path integrals. Feynman Diagram is a graphical way to represent Taylor expansion. We can expand

$$\exp\left[i\int dt\mathcal{L}\right] = \exp\left[i\int dt\mathcal{L}_0\right]\left(1 - i\int dt\frac{\lambda}{4!}x^4 + \cdots\right) \tag{99}$$

As an example, we will compute the four point function

$$\langle\Omega\left|T\hat{x}_1\hat{x}_2\hat{x}_3\hat{x}_4\right|\Omega\rangle = \lim_{T\to\infty(1-i\epsilon)} \frac{\int \mathcal{D}x\ x\left(t_1\right)x\left(t_2\right)\cdots x\left(t_n\right)e^{i\int_{-T}^{T}dt\ \mathcal{L}(t)}}{\int \mathcal{D}x\ e^{i\int_{-T}^{T}dt\ \mathcal{L}(t)}} \tag{100}$$

When $\lambda = 0$, the unperturbed four point function can be calculated using Wick's theorem in equation 97. The unperturbed 4-point function is represented as:



$$= G_{13}G_{24} + G_{12}G_{34} + G_{14}G_{23} \tag{101}$$

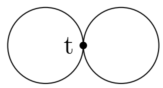
The four vertexes in each graph are t_1, t_2, t_3, t_4 respectively. The order of the vertexes are not important in this example, but you can assume the order as labeled.
When $\lambda \neq 0$, Wick theorem no longer holds because it is proven only for the harmonic oscillator Lagrangian. The idea is to express it using harmonic oscillator Lagrangian by

$$\begin{aligned}
&\langle\Omega\left|T\hat{x}_1\hat{x}_2\hat{x}_3\hat{x}_4\right|\Omega\rangle \\
&= \lim_{T\to\infty(1-i\epsilon)} \frac{\int \mathcal{D}x\ x(t_1)x(t_2)x(t_3)x(t_4)e^{i\int_{-T}^{T}dt\ \mathcal{L}(t)}}{\int \mathcal{D}x\ e^{i\int_{-T}^{T}dt\ \mathcal{L}(t)}} \\
&= \lim_{T\to\infty(1-i\epsilon)} \frac{\int \mathcal{D}x\ x(t_1)x(t_2)x(t_3)x(t_4)e^{i\int_{-T}^{T}dt\ L_0+L_1}}{\int \mathcal{D}x\ e^{i\int_{-T}^{T}dt\ \mathcal{L}_0(t)}} \frac{\int \mathcal{D}x\ e^{i\int_{-T}^{T}dt\ \mathcal{L}_0(t)}}{\int \mathcal{D}x\ e^{i\int_{-T}^{T}dt\ \mathcal{L}_0+\mathcal{L}_1}} \\
&= \lim_{T\to\infty(1-i\epsilon)} \frac{\left\langle 0\left|T\hat{x}_I(t_1)\hat{x}_I(t_2)\hat{x}_I(t_3)\hat{x}_I(t_4)e^{-\frac{i\lambda}{4!}\int_{-T}^{T}dt\ \hat{x}_I^4(t)}\right|0\right\rangle}{\left\langle 0\left|Te^{-\frac{i\lambda}{4!}\int_{-T}^{T}dt\ \hat{x}_I^4(t)}\right|0\right\rangle}
\end{aligned} \tag{102}$$

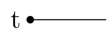
where $L_1 = -\frac{\lambda}{4!}x^4$. The state $|0\rangle$ is the vacuum for harmonic oscillator Lagrangian L_0 and the state $|\Omega\rangle$ is the vacuum for the interacting Lagrangian L.[11] Now let's look at the first order correction in the denominator[12]:

$$\left\langle 0 \left| T e^{-\frac{i\lambda}{4!}\int_{-T}^{T} dt\ \hat{x}_I^4(t)} \right| 0 \right\rangle = \langle 0| T \left\{ 1 - \frac{i\lambda}{4!}\int_{-T}^{T} dt\ \hat{x}_I^4(t) + \cdots \right\} |0\rangle$$

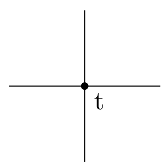
$$= 1 + \frac{1}{8}(-i\lambda)\int_{-T}^{T} dt\ G(t,t)G(t,t) \qquad (103)$$

$$= 1 + \frac{1}{8}$$ 

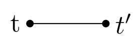
where the vertex is represented by the Feynman rules:



$$= 1 \qquad (104)$$



$$= -i\lambda \int_{-T}^{T} dt \qquad (105)$$



$$= G(t, t') \qquad (106)$$

In a Feynman diagram, each $\hat{x}(t)$ lies on a vertex t, but there can be multiple $\hat{x}(t)$ that lie on the same vertex, if the correlation function contains terms like $\hat{x}^n(t)$.

In 104, external vertex (vertex that does not come from $e^{-\frac{i\lambda}{4!}\int_{-T}^{T} dt\ \hat{x}^4(t)}$, like $\hat{x}(t_1), \hat{x}(t_2), \hat{x}(t_3), \hat{x}(t_4)$ in eq. 102) has a single edge and has value 1. In 105, each (internal) vertex has four edges and has value $-i\lambda\int_{-T}^{T} dt$. In 106, an edge that connect two vertexes is a propagator with value $G(t, t')$.

In a Feynman diagram for this theory, only these four components can appear (for example, you can't have 3 edges connecting to a single vertex), and each edge must connect two vertexes, either internal or external.

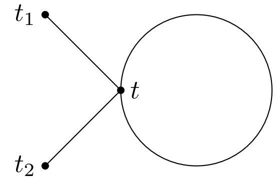
9.1 Exercise (6 pts)

Write down expressions for the following diagrams: (you don't have to evaluate the integrals)

[11] This is a very subtle difference and not very important for the present discussion. Intuitively, vacuum is the lowest energy state, so if you change the Lagrangian from L_0 to L_1, the state that has lowest energy under L_0 will not have the lowest possible energy in L_1, so the vacuum state will change.

[12] (For more advanced readers) For simplicity I have excluded the symmetry factors in the expressions of Feynman diagrams, and instead divide out the symmetry factor (8 in the next equation) as a weight outside.

(i)

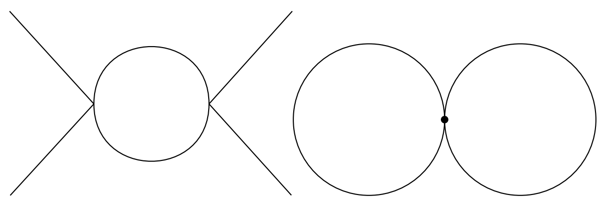


(107)

Answer:

$$-i\lambda \int_{-T}^{T} dt\ G(t_1,t)G(t,t_2)G(t,t) \tag{S81}$$

(ii) The following is a *disconnected* diagram, so you should write down expressions for each connected component and multiply together. (Label the vertexes yourself)



(108)

Answer: Label the four external vertexes $t_1, t_2; t_3, t_4$ from left to right. The three internal vertexes are t, t', t'' from left to right.

$$i\lambda^3 \int_{-T}^{T} dt \int_{-T}^{T} dt' G(t,t_1)G(t,t_2)G(t,t')^2 G(t',t_3)G(t',t_4) \times \int_{-T}^{T} dt'' G(t'',t'')^2 \tag{S82}$$

9.2 Exercise (4 pts)

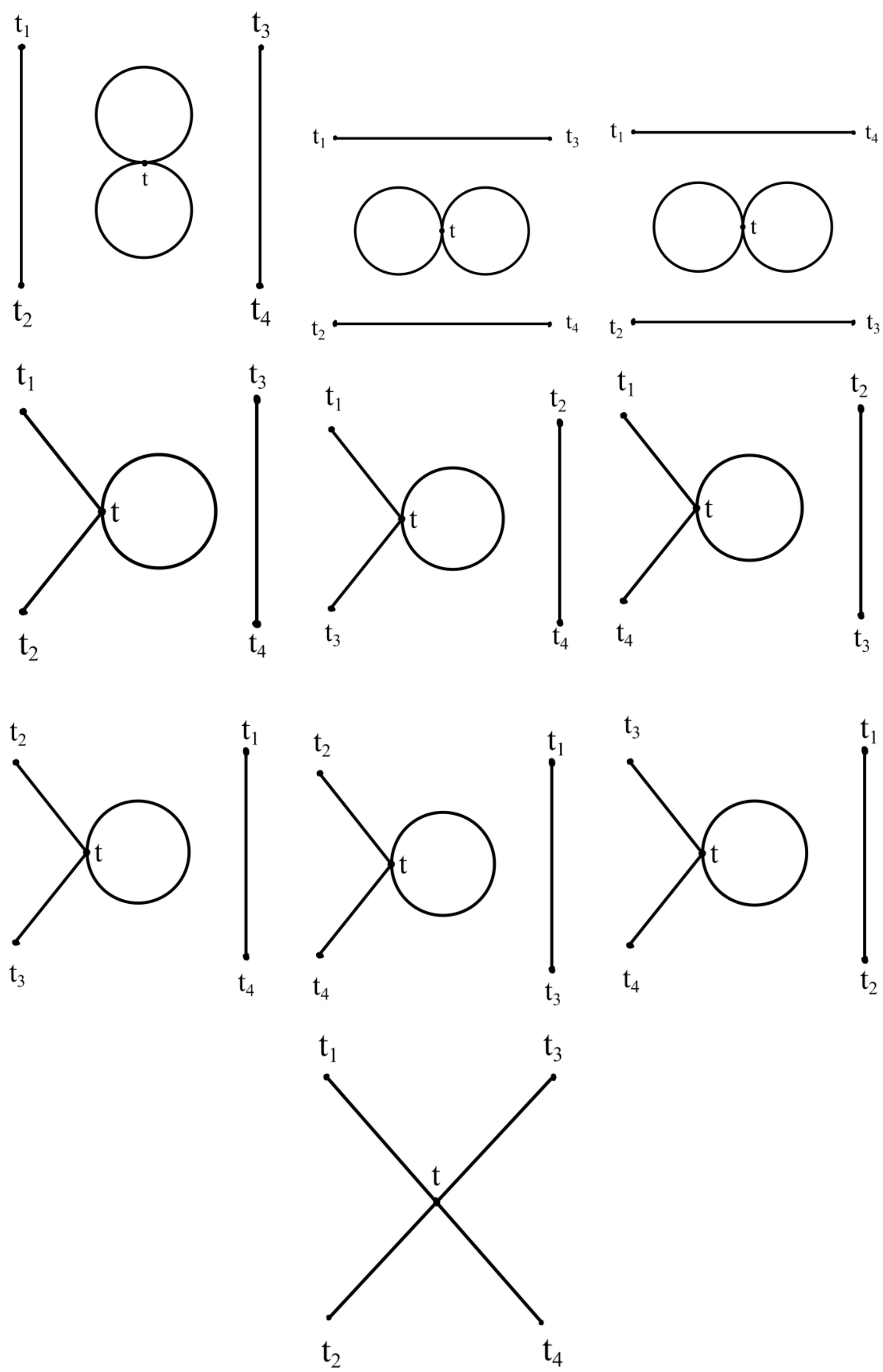
Write down Feynman diagrams and its expressions of the first order correction (in λ) in the numerator of four point function eq 102:

$$\left\langle 0 \left| T\hat{x}_I(t_1)\hat{x}_I(t_2)\hat{x}_I(t_3)\hat{x}_I(t_4)\left(-\frac{i\lambda}{4!}\right)\int_{-T}^{T} dt\ \hat{x}_I^4(t) \right| 0 \right\rangle \tag{109}$$

You don't have to evaluate the integrals. Hint: every diagram has four external vertexes, one internal vertex, and four edges. Remember the diagrams can be disconnected.

Answer: [13]

[13] This answer is revised from team AceD's answer.


t_1 t_2 t t_3 t_4
t_1 t_3 t t_2 t_4
t_1 t_4 t t_2 t_3
t_1 t t_2 t_3 t_4
t_1 t t_3 t_2 t_4
t_1 t t_4 t_2 t_3
t_2 t t_3 t_1 t_4
t_2 t t_4 t_1 t_3
t_3 t t_4 t_1 t_2
t_1 t_3 t t_2 t_4

The expressions for the diagrams are given by

$$D_1 = -i\lambda \int dt G(t_1, t_2) G(t_3, t_4) G(t,t) G(t,t)$$

$$D_2 = -i\lambda \int dt G(t_1, t_3) G(t_2, t_4) G(t,t) G(t,t)$$

$$D_3 = -i\lambda \int dt G(t_1, t_4) G(t_2, t_3) G(t,t) G(t,t)$$

$$D_4 = -i\lambda \int dt G(t_1, t) G(t_2, t) G(t,t) G(t_3, t_4)$$

$$D_5 = -i\lambda \int dt G(t_1, t) G(t_3, t) G(t,t) G(t_2, t_4)$$

$$D_6 = -i\lambda \int dt G(t_1, t) G(t_4, t) G(t,t) G(t_2, t_3)$$

$$D_7 = -i\lambda \int dt G(t_2, t) G(t_3, t) G(t,t) G(t_1, t_4)$$

$$D_8 = -i\lambda \int dt G(t_2, t) G(t_4, t) G(t,t) G(t_1, t_3)$$

$$D_9 = -i\lambda \int dt G(t_3, t) G(t_4, t) G(t,t) G(t_1, t_2)$$

$$D_{10} = -i\lambda \int dt G(t_1, t) G(t_2, t) G(t, t_3) G(t, t_4)$$

Thus, the total contribution of this term will be

$$\left\langle 0 \middle| T \left\{ \hat{x}_I(t_1) \hat{x}_I(t_2) \hat{x}_I(t_3) \hat{x}_I(t_4) \left(-\frac{i\lambda}{4!}\right) \int_{-T}^{T} dt\ \hat{x}_I^4(t) \right\} \middle| 0 \right\rangle$$
$$= s_1(D_1 + D_2 + D_3) + s_2(D_4 + \ldots + D_9) + s_3 D_{10}$$

where the s_i are *one over* the symmetry factor for each diagram. But you don't need to know what symmetry factor is: you can count the factors from Wick's theorem. From eq. 103, we know $s_1 = \frac{3}{4!} = \frac{1}{8}$. The diagrams $4 \ldots 9$ all have one loop and $s_2 = \frac{4 \times 3}{4!} = \frac{1}{2}$. The last diagram has no loop, so s_3 is $\frac{4!}{4!} = 1$.

9.3 Exercise (4 pts)

Put your result in section 9.2 and eq 103 back to eq. 102, do you see $G_{13}G_{24} + G_{12}G_{34} + G_{14}G_{23}$ appearing in your first-order expression?

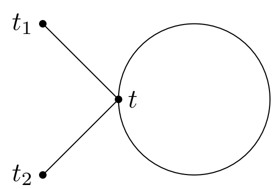
Answer: Put in the zeroth order and first order (in λ) of the numerator in eq. 102, and uses eq. 103:

$$
\begin{aligned}
&\langle\Omega\,|T\hat{x}_1\hat{x}_2\hat{x}_3\hat{x}_4|\,\Omega\rangle \\
=&\frac{G_{13}G_{24}+G_{12}G_{34}+G_{14}G_{23}+\frac{1}{8}\left(D_1+D_2+D_3\right)+\frac{1}{2}\left(D_4+\ldots+D_9\right)+D_{10}}{1+\frac{1}{8}(-i\lambda)\int_{-T}^{T}dt\;G(t,t)G(t,t)} \\
=&G_{13}G_{24}+G_{12}G_{34}+G_{14}G_{23}+\frac{\frac{1}{2}\left(D_4+\ldots+D_9\right)+D_{10}}{1+\frac{1}{8}(-i\lambda)\int_{-T}^{T}dt\;G(t,t)G(t,t)}
\end{aligned}
$$

So $G_{13}G_{24}+G_{12}G_{34}+G_{14}G_{23}$ does appear. To look at other terms we need to go to higher orders.

9.4 Exercise (3 pts)

Evaluate the following diagram when $t_1=t_2=0$ using eq 98, at $T\to\infty(1-i\epsilon)$ limit.



(110)

Answer:

$$
\begin{aligned}
&-i\lambda\int_{-T}^{T}dt\;G(t,t_1)G(t,t_2)G(t,t)\Big|_{t_1=t_2=0} \\
=&-i\lambda\int_{-T}^{T}dt\;\frac{1}{8\omega^3}e^{-2i\omega|t|} \\
=&-\frac{i\lambda}{4\omega^3}\int_0^T dt\;e^{-2i\omega t} \\
=&\frac{\lambda}{8\omega^4}e^{-2i\omega t}\Big|_{t=0}^{T} \\
=&-\frac{\lambda}{8\omega^4}
\end{aligned}
$$

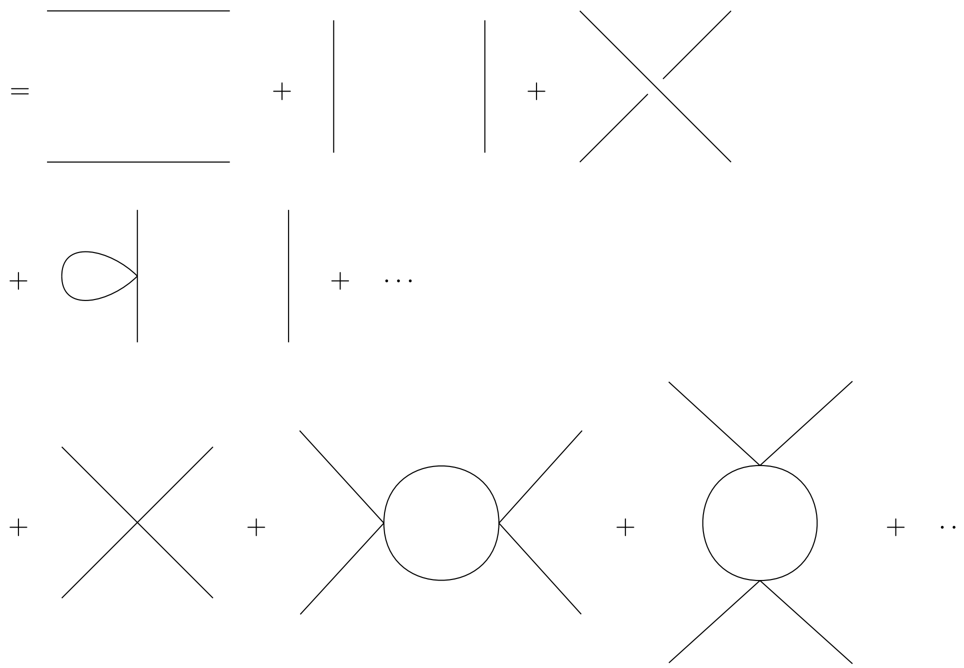
where in passing to the last line we have used

$$
\lim_{T\to\infty(1-i\epsilon)}e^{-2i\omega t}=\lim_{a\to\infty}e^{-2i\omega a(1-i\epsilon)}=0 \quad \text{(S83)}
$$

The $-i\epsilon$ term makes the integral convergent. One could argue that the notation here is confusing: $|t|$ can also be interpreted as the norm of a complex number, so $-i\epsilon$ term has no effect. I apologize for this possible confusion.

Generally, as you may have guessed,

$$\langle\Omega\left|T\left[\hat{x}\left(t_1\right)\hat{x}\left(t_2\right)\hat{x}\left(t_3\right)\hat{x}\left(t_4\right)\right]\right|\Omega\rangle=\left(\begin{array}{c}\text{sum of all connected diagrams}\\ \text{with 4 external points}\end{array}\right)$$



(111)

where "disconnected" means "disconnected from all external points" and external points can be disconnected from each other. The reason only connected diagrams contribute is because the denominator in eq. 83 cancels out diagrams that are not connected to any external points. In the equation above each diagram comes with the appropriate combinatoric factor: one over the symmetry factor of the diagram. The symmetry factor is the number of symmetries of a diagram, since symmetries reduce the number of Wick contractions. In most textbooks, the calculation of Feynman diagram is defined to be divided by its symmetry factor in the end. I did not define the calculation to include this because it is very hard to count the correct symmetry factor.

You might be wondering why we are calculating correlation functions in the first place. The reason is that we can calculate scattering amplitudes from correlation functions, and scattering amplitudes can be measured in collider experiments. Of course, there are much more useful and efficient ways of calculating scattering amplitudes in quantum mechanics, and people rarely use path integral to calculate scattering amplitudes in QM, but the formalism we have introduced in the last two sections carry directly to *quantum field theory*. Our most precise theories of electromagnetic, weak, and strong interactions are all quantum field theories. I am not going to delve deep into scattering amplitudes or quantum field theory, but you should keep in mind that the proofs you have worked out in the last two sections can be carried directly to quantum field theory with little modifications.