Physics Unlimited Explorer Competition 2022

Assignment packet, rev. 2

Submissions due: May 1, 2022 11:59 pm EST (plus 3-hour grace period)

Guidelines

Student teams are given **up to four weeks** to work on the 2022 Explorer Competition, and teams registering later than the assignment release date may begin work at any time. Please refer to the sections below for details on both formatting and the submission process.

Scoring

Students are encouraged to work on as much of the assignment as possible. The award structure will be as follows:

1. Certificate awards will be given to the four teams with the highest scores, per scoring rubric that would allocate points for questions and exercises based on their difficulty level as determined by the assignment creator.
2. There will be medalist-level certificates granted for first place, second place, and third place, respectively (or tied teams, if applicable).
3. There will be an honorable mention certificate granted to the fourth-highest scoring submission (or tied teams, if applicable).

Collaboration Policy and External Resources

Students participating in the competition **may only correspond with members of their team**. Absolutely and unequivocally, **no other form of human correspondence is allowed**. This includes any form of correspondence with mentors, teachers, professors, and other students. Participating students are barred from posting content or asking questions related to the exam on the internet (except where specified below), and moreover, they are unequivocally barred from seeking the solution to any of the exams' parts from the internet or another resource. Students are allowed, however, to use the following resources for purposes of reference and computation:

- **Internet**: Teams may use the internet for purposes of reference with appropriate citation. For information about appropriate citation, see below.

- **Books and Other Literature**: Teams may use books or other literature, in print or online, for purposes of reference with appropriate citation. As with the use of the Internet, teams are in no way allowed to seek the solution to any of the exams' parts from books or other literature.
- **Computational Software**: Teams may use computational software, e.g. Mathematica, Matlab, Python, whenever they deem it appropriate. Of course, teams must clearly indicate that they have used such software. Additionally, the judges reserve to right to deduct points for the use of computational software where the solution may be obtained simply otherwise.

Citation

All student submissions that include outside material must include numbered citations. We do not prefer any style of citation in particular.

Submission

Team assignment

All submissions, regardless of formatting, **should include a cover page listing the title of the work, the date, and electronic or scanned signatures of all team participants**. The work must be submitted as a single **PDF document** with the ".pdf" extension. All other formatting decisions are delegated to the teams themselves. No one style is favored over another. That being said, we recommend that teams use a typesetting language (e.g. LATEX) or a word-processing program (e.g. Microsoft Word, Pages). **Handwritten solutions are allowed**, but we reserve the right **to refuse grading of any portion of a team's submission in the case that the writing or solution is illegible**.

All teams must submit their solutions to PUEC 2022 by emailing **directors@physicsu.org by 11:59 pm U.S. Eastern Time (UTC-5) on Sunday, May 1, 2022**. Teams will not be able to submit their solutions to the Explorer Competition at any later time, barring exceptional circumstances related to technical issues (granted on a case-by-case basis), with a no-excuse-needed grace period of three hours after the deadline.

Only the team member who submitted the team registration form should send the submission; in case they are unable to, another team member may do so. The title of the submission e-mail should be formatted as **PUEC 2022 SUBMISSION: Team Name**, where **Team Name** is to be replaced with your actual team's name, as officially registered. All teams may make multiple submissions. However, we will **only download, read and grade the most recent submission emailed to us using the requested format before the deadline**. Teams will receive confirmation once their submission has been received within at most three days. **In the case of extraordinary circumstances, please contact us as soon as possible**.

Individual form and fee

Each team member in every team is expected to submit an **individual feedback form** prior to the team submission deadline, where they will have the opportunity to also self-report the approximate fraction of their contribution to the team's work. Each participant is welcome to contribute an amount commensurate with their situation, to be reported through this form. Invoices will be emailed based on the individual responses to this form within a week of their receipt.

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.)

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.

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

1.3 Exercise (2 pts)

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

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 $x(t_b) = x_b$.

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

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

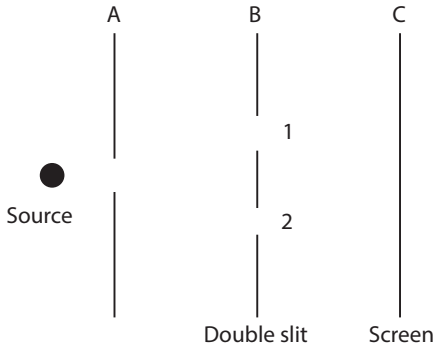
does not change with time.
Hence, show that if the potential energy does not depend on velocity or time explicitly, the Hamiltonian equals the sum of kinetic and potential energy.

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

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

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

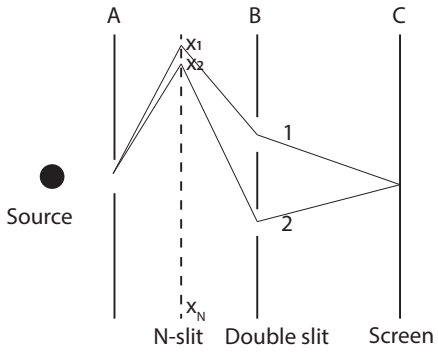
where $\Phi(x)$ is a complex number called the probability amplitude. Let Φ_1 and Φ_2 be the amplitudes when electrons pass through slit 1 and 2 respectively. The principle of superposition says the probability amplitudes add up linearly

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

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 $\hbar$.

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.

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.

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

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:

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

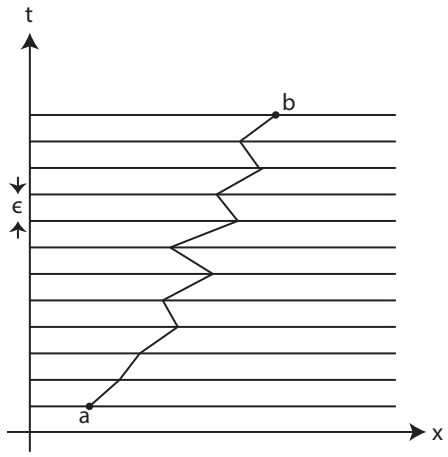
[1]This set of postulates is far from complete. See section 2.7 for more postulates. The only change from the usual Schrödinger picture's postulates is that the time evolution of wave function follows path integral representation, not Schrödinger's function.

2.3.1 Exercise (1 pts)

Discuss the physical meaning of the constancy of C in all different paths.

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.

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

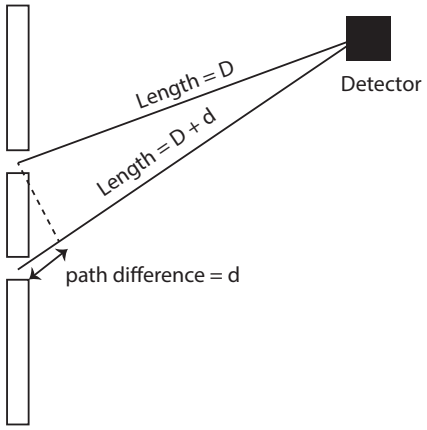
The path integral is defined as

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

2.4.1 Exercise (1 pts)

Show your argument that A is function of ϵ.

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.

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).

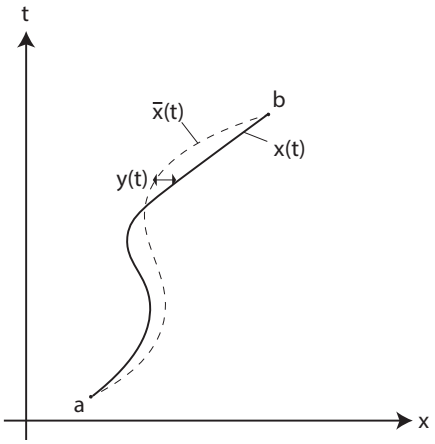
2.6 Technique in doing Path Integral

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:

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

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: $\int_{-\infty}^{\infty} e^{-x^2}dx = \sqrt{\pi}$

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

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:* $\langle\psi|\psi\rangle = 1$.

2.7.3 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.

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.

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.

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 $V(x_0 + \frac{\delta x}{2})$.

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. 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:

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

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

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

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.

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.

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.

5.4 Exercise (4 pts)

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

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

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.

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.

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

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

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

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

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 $\delta y = \frac{df(x)}{dx}\delta x$)

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

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

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 $dS = \frac{dQ}{T}$)

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.

7 Path Integral Calculation of Partition Function

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

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

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

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

7.2 Exercise (5 pts)

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

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.

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:

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

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.[4]. 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:

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

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** $x(T) = x_b$[5]. Break up the functional integral into three parts:

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

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

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

[4]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.

[5]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.

8.2 Exercise (4 pts)

Prove

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

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

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

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

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*:

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

8.3 Exercise (4 pts)

Prove

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

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

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

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

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

and

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

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:

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

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.

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.

9 Feynman Diagram

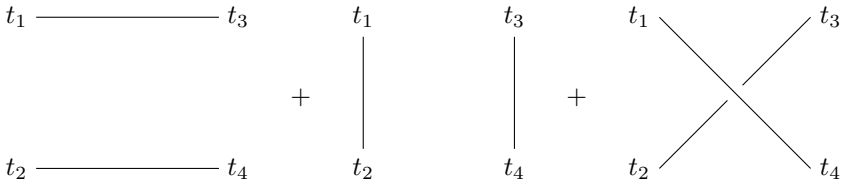
Now we add a small perturbation to the harmonic oscillator Lagrangian L_0: $\mathcal{L} = \mathcal{L}_0 - \frac{\lambda}{4!}x^4$. In this example the theory can still be analytically solved, but in general the theory becomes unsolvable (no analytic expression). We will assume $\lambda \ll 1$ and use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



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

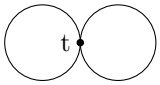
The four vertexes in each graph are t_1, t_2, t_3, t_4 respectively. The order of the vertexes are not important in this example, but you can assume the order as labeled.

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

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

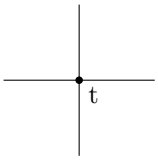
where $L_1 = -\frac{\lambda}{4!}x^4$. The state $|0\rangle$ is the vacuum for harmonic oscillator Lagrangian L_0 and the state $|\Omega\rangle$ is the vacuum for the interacting Lagrangian L.[6] Now let's look at the first order correction in the denominator[7]:

$$\begin{aligned}
&\left\langle 0 \left| T e^{-\frac{i\lambda}{4!}\int_{-T}^{T} dt\ \hat{x}_I^4(t)} \right| 0 \right\rangle = \langle 0|T\left\{1 - \frac{i\lambda}{4!}\int_{-T}^{T} dt\ \hat{x}_I^4(t) + \cdots\right\}|0\rangle \\
&= 1 + \frac{1}{8}(-i\lambda)\int_{-T}^{T} dt\ G(t,t)G(t,t) \qquad (103) \\
&= 1 + \frac{1}{8}
\end{aligned}$$

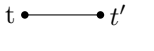


where the vertex is represented by the Feynman rules:

$$= 1 \qquad (104)$$



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



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

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.

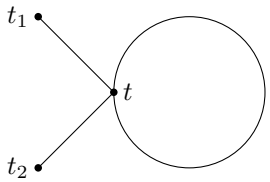
9.1 Exercise (6 pts)

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

[6] 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.

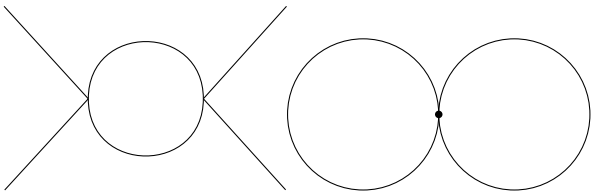
[7] (For more advanced readers) For simplicity I have excluded the symmetry factors in the expressions of Feynman diagrams, and instead divide out the symmetry factor (8 in the next equation) as a weight outside.

(i)



(107)

(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)

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:

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

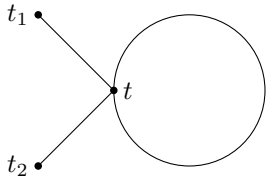
You don't have to evaluate the integrals. Hint: every diagram has four external vertexes, one internal vertex, and four edges. Remember the diagrams can be disconnected.

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?

9.4 Exercise (3 pts)

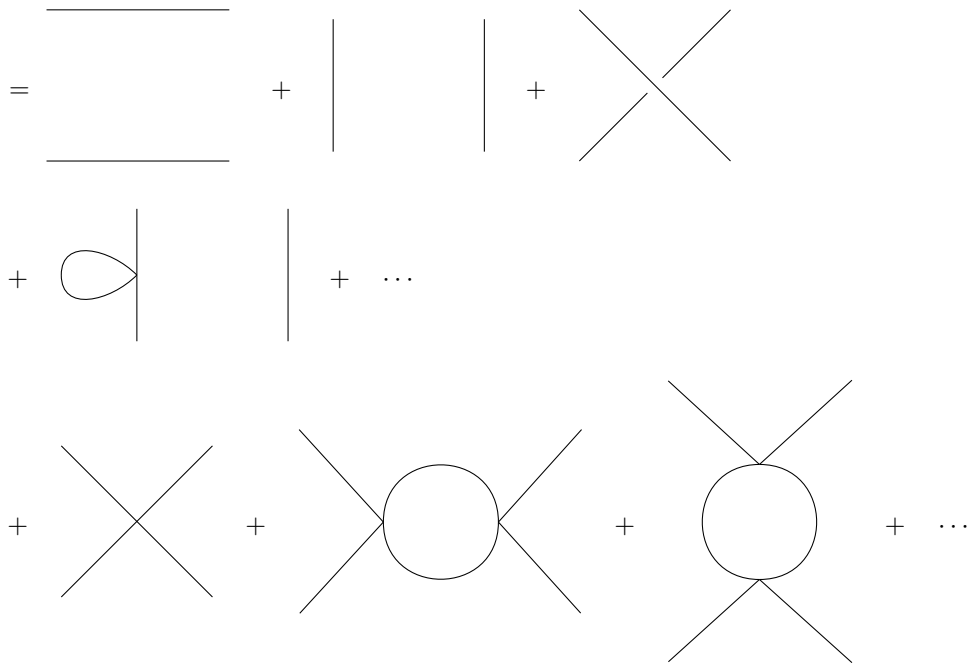
Evaluate the following diagram when $t_1 = t_2 = 0$ using eq 98, at $T \to \infty(1 - i\epsilon)$ limit.



(110)

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.

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.