# Path Integrals

Selected chapter of lecture notes on Quantum Mechanics

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## Contents

# 1 Introduction. Historical Remarks

The founders of quantum mechanics developed its formalism generalizing the formulation of classical mechanics in which physical system dynamics is followed as a function of time. Given the state of the system at some time differential equations gave its state at the next moment and so on. Classically this description was based on the Hamilton function of canonical coordinates and momenta. In quantum mechanics the Hamilton function and canonical variables become operators used in Schrödinger or Heisenberg equations controlling the time development of the system. This way of going from classical to quantum mechanical description in a given physical system is often called canonical quantization.

Path integral formulation of quantum mechanics can be viewed as an extension of the classical action principle approach. This formulation was developed by Richard Feynman when he was looking for how to quantize the version of classical electrodynamics which he and Wheeler developed. It is presently called Wheeler–Feynman absorber theory of electrodynamics, cf., Ref. [1]. The reader is welcome to read Feynman's Nobel Lecture, Ref. [2] for his personal story of this and the discoveries which followed, cf., Ref. [3].

In the classical action principle approach one addresses the properties, the character of the entire path of the physical system throughout the space and time between given initial and final configurations. The basis of this approach is a statement that a physical system moves between initial and final coordinate configurations from initial to final times $t_i$, $t_f$,

$$q_i, t_i \to q_f, t_f \tag{1}$$

along such a path that a certain functional of all paths $S[path]$ satisfying Eq. (1) and called action is stationary. Mathematically this means that its 1st variation vanishes $\delta S = 0$. The standard classical expression for $S[path]$ is via the system Lagrangian

$$S[path] \equiv S[q(t)] = \int_{t_i}^{t_f} L(q, \dot{q}) dt \tag{2}$$

Quantum mechanical path integral formulation replaces the classical path choice by stating that all possible paths are allowed between initial and final configurations each with the probability amplitude

$$K(q_f, t_f; q_i, t_i; path) = const\, e^{iS[path]/\hbar} \tag{3}$$

Each such amplitude is considered as independent so that following the rules of quantum mechanics the entire probability amplitude is given by the sum over all possible paths, i.e. the path integral

$$K(q_f, t_f; q_i, t_i) = \int D[path]\, e^{iS[path]/\hbar} \tag{4}$$

In the rest of this Chapter we will provide mathematically more precise definition of the above expression, its relation to the canonical quantization formalism and explore simple examples of its application, cf., Refs. [4, 5].

# 2 Path Integrals - The Basics

## 2.1 From canonical quantization to path integrals

### 2.1.1 The propagator

The bi-local function $K(q_f, t_f; q_i, t_i)$ in the path integral expression Eq. (4) is called quantum mechanical propagator. It is useful to recognize that it is actually a wave function at time $t_f$

$$\Psi(q_f, t_f) \equiv \langle q_f | \Psi(t_f) \rangle \tag{5}$$

satisfying the following initial condition at time $t_i$

$$\Psi(q, t_i) \equiv \langle q | \Psi(t_i) \rangle = \langle q | q_i \rangle = \delta(q - q_i) \tag{6}$$

Writing the Schrödinger equation for this $|\Psi(t)\rangle$

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H_{op} |\Psi(t)\rangle \tag{7}$$

assuming the most common case of the time independent $H_{op}$ and using the formal solution of this equation

$$|\Psi(t)\rangle = e^{-iH_{op}(t-t_i)/\hbar} |\Psi(t_i)\rangle \tag{8}$$

with initial condition $|\Psi(t_i)\rangle = |q_i\rangle$ we obtain

$$K(q_f, t_f; q_i, t_i) = \langle q_f | \Psi(t_f) \rangle = \langle q_f | e^{-iH_{op}(t_f - t_i)/\hbar} | q_i \rangle \tag{9}$$

So the propagator is a coordinate space matrix element of the time evolution operator

$$U(t_f, t_i) = e^{-iH_{op}(t_f - t_i)/\hbar} \tag{10}$$

Note that this is correct for the Hamiltonian $H_{op}$ which is independent on time. We will discuss below how this is modified for time dependent $H_{op}(t)$.

For any wave function $\Psi(q, t')$ at a time $t'$ the propagator allows to determine how this wave function propagates over a finite time $t - t'$

$$\Psi(q, t) = \int dq' K(q, t; q', t') \Psi(q', t') \tag{11}$$

Let us note that for the time independent Hamiltonians $H_{op}$ which we are considering the propagator can be expressed in terms of the eigenfunctions

$$H_{op} |\psi_m\rangle = E_m |\psi_m\rangle \tag{12}$$

Inserting compete sets of $|\psi_n\rangle$ in the expression Eq. (9) we obtain

$$\begin{aligned} K(q_f,t_f;q_i,t_i) &= \sum_{m,n}\langle q_f|\psi_m\rangle\langle\psi_m|e^{-iH_{op}(t_f-t_i)/\hbar}|\psi_n\rangle\langle\psi_n|q_i\rangle = \\ &= \sum_m \psi_m(q_f)\psi_m^*(q_i)e^{-iE_m(t_f-t_i)/\hbar} \end{aligned} \tag{13}$$

This relation as well as Eq. (11) show that the propagator contains the information of essentially all solutions of the Schrödinger equation. This information is "encoded" in the dependence of $K(q_f,t_f;q_i,t_i)$ on two coordinate-time pairs $q_i,t_i$ and $q_f,t_f$.

Let us also note that the following "composition law" holds for the propagators

$$K(q,t;q'',t'') = \int K(q,t;q',t')K(q',t';q'',t'')dq' \tag{14}$$

which is quite obvious from the operator form Eq. (9). It is this relation used many times which will form the basis of the path integral approach as will be developed below.

### 2.1.2 Relation to the Green's function

Let us note that the propagator as defined above is in a very simple way related to the Green's function of the Schrödinger equation. All one needs is to restrict it to e.g. positive evolution times[1]. Writing this formally using the step function $\theta(t-t')$ one defines

$$G(q,t;q',t') = \frac{1}{i\hbar}\theta(t-t')K(q,t;q',t') \tag{15}$$

or in the operator form

$$\hat{G}(t,t') = \frac{1}{i\hbar}\theta(t-t')e^{-iH_{op}(t-t')/\hbar} \tag{16}$$

Acting on $\hat{G}$ with $i\hbar\partial_t - H_{op}$ and using Eq. (10) gives

$$\left(i\hbar\frac{\partial}{\partial t} - H_{op}\right)\hat{G}(t,t') = \delta(t-t') \tag{17}$$

or in the coordinate representation

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}_q\right)G(q,t;q',t') = \delta(t-t')\delta(q-q') \tag{18}$$

[1]One can also use negative evolution times $-(1/i\hbar)\theta(t'-t)K(q,t;q',t')$ or linear combinations of the both.

where we used $\lim_{t\to t'} K(q,t;q',t') = \delta(q-q')$ which follows from Eq. (6) and denoted $\hat{H}_q$ for $H_{op}$ in the coordinate representation, i.e.

$$\langle q|H_{op}|\Psi\rangle = \int dq''\langle q|H_{op}|q''\rangle\langle q''|\Psi\rangle \equiv \hat{H}_q\langle q|\Psi\rangle$$

We note that the above equations for $G$ are indeed equations for the Green's function of the time dependent Schrödinger equation.

For time independent Hamiltonians which we are considering the propagator (9) dependence on the initial and final times $t$ and $t'$ is via the difference $T = t - t'$. This makes it useful to consider the energy dependent Green's function

$$G(q,q';E) = \frac{1}{i\hbar}\int_0^\infty dT e^{(i/\hbar)ET} K(q,T;q',0) = \sum_m \frac{\psi_m(q)\psi_m^*(q')}{E - E_m + i0} \tag{19}$$

where the $i0$ term in the denominator is a conventional notation for an infinitesimally small imaginary part of $E$ needed to make the above integral converge at $T \to \infty$.

Let us act with $(E - \hat{H}_q)$ on both sides of the above expression. Using stationary Schrödinger equation (12) and the completeness relation $\sum_m \psi_m(q)\psi_m^*(q') = \delta(q-q')$ we obtain

$$(E - \hat{H}_q)G(q,q';E) = \delta(q-q') \tag{20}$$

showing that (as expected) $G(q,q';E)$ is a Green's function of the stationary Schrödinger equation. Its formal expression clearly follows from the opertor form of the above equation

$$(E - H_{op})\hat{G}(E) = \hat{1} \quad \to \quad \hat{G}(E) = (E - H_{op} + i0)^{-1} = \frac{1}{i\hbar}\int_0^\infty dT\, e^{-iH_{op}T/\hbar} \tag{21}$$

matching the definitions in Eq. (16). In the context of this Chapter this Green's function will be useful in discussions and applications of the semiclassical limit of the path integral formalism.

### 2.1.3 Free particle

Let us calculate the propagator for a free particle moving in one dimension. In this case the system coordinates are $q \to x$ and the Hamiltonian is

$$H_{op} = \frac{p_{op}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \tag{22}$$

The propagator can be calculated by using momentum eigenstates

$$p_{op}|p>=p|p> \quad \rightarrow \quad H_{op}|p\rangle = \frac{p^2}{2m}|p\rangle \tag{23}$$

which diagonalize this Hamiltonian.

Inserting the relation $\int dp|p><p| = 1$ for the complete set of such states

$$K(x,t;x',t') = \langle x|e^{-i(p_{op}^2/2m)(t-t')/\hbar}|x'\rangle = \int dp\langle x|e^{-i(p_{op}^2/2m)(t-t')/\hbar}|p\rangle\langle p|x'\rangle \tag{24}$$

we obtain

$$K(x,t;x',t') = \int dp\, e^{-i(p^2/2m)(t-t')/\hbar}\langle x|p\rangle\langle p|x'\rangle = \int \frac{dp}{2\pi\hbar}\exp\{\frac{i}{\hbar}[p(x-x')-\frac{p^2}{2m}(t-t')]\}$$

where in the last step we used the explicit form of the momentum eigenstates in the x-representation

$$<x|p>=\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$$

The $dp$ integral in above expression for $K(x,t;x',t')$ belongs to the Gaussian integrals which are analytically calculable, cf., Appendix, Section 5.1, and one obtains

$$K(x,t;x',t') = \sqrt{\frac{m}{2\pi i\hbar(t-t')}}\exp\left[\frac{i}{\hbar}\frac{m(x-x')^2}{2(t-t')}\right] \tag{25}$$

There are many interesting features in the behaviour of this expression at large and small distances $x-x'$ and large and small time intervals $t-t'$, cf. Ref. [6] for details.

Let us note that using the above expression it is straightforward to write the propagator for a free particle in three dimensions $\mathbf{r} = (x,y,z)$

$$K(\mathbf{r},t;\mathbf{r}',t') = \left[\frac{m}{2\pi i\hbar(t-t')}\right]^{3/2}\exp\left[\frac{i}{\hbar}\frac{m(\mathbf{r}-\mathbf{r}')^2}{2(t-t')}\right] \tag{26}$$

The free particle is one of the few examples for which the propagator can be evaluated explicitly. Another is the propagator for harmonic oscillator which we will derive below using path integrals.

### 2.1.4 Configuration space path integral. One dimension

The exponential form of the time evolution operator Eq. (10) allows to represent the time propagation of the corresponding physical system between initial and final times as a sequence of intermediate time steps. Choosing for convenience $N$ time steps with equal time lengths

$$\epsilon = \frac{t_f - t_i}{N} \tag{27}$$

writing $U(t_f, t_i)$ in Eq. (9) as a product of evolutions over the steps and inserting complete sets of coordinate states

$$\int |q_n\rangle\langle q_n| dq_n = 1 \quad , \quad n = 1, ..., N-1$$

at each step we obtain

$$K(q_f, t_f; q_i, t_i) = \langle q_f | \underbrace{e^{-iH_{op}\epsilon/\hbar} ..... e^{-iH_{op}\epsilon/\hbar}}_{N\, times} | q_f \rangle = \tag{28}$$

$$= \int dq_1 dq_2 ... dq_{N-1} \langle q_f | e^{-iH_{op}\epsilon/\hbar} | q_{N-1} \rangle \langle q_{N-1} | e^{-iH_{op}\epsilon/\hbar} | q_{N-2} \rangle \ldots \langle q_1 | e^{-iH_{op}\epsilon/\hbar} | q_i \rangle$$

This expression provides the formal basis for the path integral approach. It shows that the probability amplitude to propagate from $q_i, t_i$ to $q_f, t_f$ can be viewed as a sum of amplitudes to propagate in $N$ time intervals $\epsilon$ through all possible sequences $q_1, ....q_{N-1}$ of $N$ intermediate points, cf., Fig. 1.

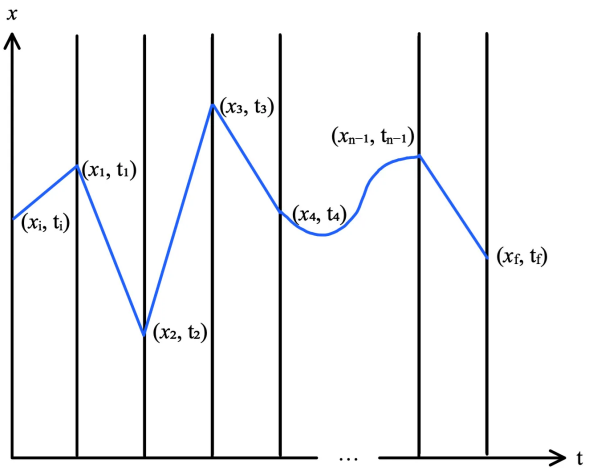


Figure 1: Schematic representation of the expression Eq. (28) as a sum of all possible propagation paths between fixed initial and final points

The final natural step is to go to the limit $N \to \infty$ or $\epsilon \to 0$. In this limit the infinitesimal propagators

$$\lim_{\epsilon \to 0} \langle q_n | e^{-iH_{op}\epsilon/\hbar} | q_{n-1} \rangle$$

between any pair $q_{n-1}, q_n$ of coordinates can be calculated for essentially any physically relevant Hamiltonian $H_{op}$. Let us start by showing this in the simple one dimensional case $q \equiv x$ with the standard Hamiltonian

$$H_{op} = \frac{p_{op}^2}{2m} + V(x_{op}) \tag{29}$$

The infinitesimal propagator is then

$$\begin{aligned} \lim_{\epsilon \to 0} \langle x_n | e^{-iH_{op}\epsilon/\hbar} | x_{n-1} \rangle &= \langle x_n | 1 - i\epsilon [p_{op}^2/2m + V(x_{op})]/\hbar + O(\epsilon^2) | x_{n-1} \rangle = \\ &= \langle x_n | [1 - (i\epsilon/\hbar) p_{op}^2/2m][1 - (i\epsilon/\hbar) V(x_{op})] + O(\epsilon^2) | x_{n-1} \rangle = \\ &= \langle x_n | e^{-(i\epsilon/\hbar)p_{op}^2/2m} e^{-(i\epsilon/\hbar)V(x_{op})} + O(\epsilon^2) | x_{n-1} \rangle \end{aligned} \tag{30}$$

We have a product of $N$ such terms in Eq. (28) so that the $O(\epsilon^2)$ parts add N times and become $O(\epsilon)$ which is negligible in the $N \to \infty$ limit. The remaining part of the propagators can then be calculated by using

$$V(x_{op}) | x_{n-1} \rangle = V(x_{n-1}) | x_{n-1} \rangle$$

which gives

$$\lim_{\epsilon\to 0}\langle x_n|e^{-iH_{op}\epsilon/\hbar}|x_{n-1}\rangle \approx \langle x_n|e^{-(i\epsilon/\hbar)p_{op}^2/2m}|x_{n-1}\rangle e^{-(i\epsilon/\hbar)V(x_{n-1})} \tag{31}$$

and then recognizing that the term with the kinetic energy is just a free particle propagator, Eq. (25). This gives

$$\lim_{\epsilon\to 0}\langle x_n|e^{-iH_{op}\epsilon/\hbar}|x_{n-1}\rangle \approx \sqrt{\frac{m}{2\pi i\hbar\epsilon}}\exp\frac{i}{\hbar}\left[\frac{m(x_n-x_{n-1})^2}{2\epsilon}-\epsilon V(x_{n-1})\right] \tag{32}$$

Using this expression in Eq. (28) with q replaced by x and taking the limit $N\to\infty$, $\epsilon\to 0$ one obtains

$$K(x_f,t_f;x_i,t_i)=\lim_{\epsilon\to 0}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}\int\prod_{n=1}^{N-1}dx_n\exp[\frac{i}{\hbar}S(x_1,...,x_{N-1})] \tag{33}$$

with

$$S(x_1,...,x_{N-1})=\sum_{n=1}^{N}\epsilon\left[\frac{m}{2}\left(\frac{x_n-x_{n-1}}{\epsilon}\right)^2-V(x_{n-1})\right] \tag{34}$$

and fixed $x_0=x_i$, $x_N=x_f$.

We recognize that the above expression for $S(x_1,...,x_{N-1})$ is a discretized version of the classical action integral

$$S[x(t)]=\int_{t_i}^{t_f}dt\left[\frac{m}{2}\left(\frac{dx}{dt}\right)^2-V(x)\right]=\int_{t_i}^{t_f}dt\;L\left(x(t),\dot{x}(t)\right) \tag{35}$$

where $L$ is the classical Lagrangian. The function $x(t)$ is a path in the coordinate space which is defined, cf., Fig. 1 for $t_i\le t\le t_f$ with intermediate points

$$x(t=t_i+n\epsilon)=x_n\quad,\quad n=1,...N-1 \tag{36}$$

which are varying integration variables each taking on all the values of the integration range $-\infty\le x_n\le\infty$ and the fixed endpoints

$$x(t_i)=x_i\quad,\quad x(t_f)\equiv x(t_i+N\epsilon)=x_f \tag{37}$$

As $N\to\infty$ the above discretized functions become continuous paths and the integral becomes a path integral over an infinite space of such paths.

The convenient compact notation for the above path integral representing the propagator is

$$K(x_f, t_f; x_i, t_i) = \int Dx(t) e^{(i/\hbar)S[x(t)]} \tag{38}$$

with the action Eq. (35) and the differential "volume" in the path integration space

$$Dx(t) \equiv \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2} \prod_{n=1}^{N-1} dx_n \tag{39}$$

There are formal limitations in regarding this expression as the rigorous formal $\epsilon \to 0$ limit of the discrete Eq. (33). One must note that the independent variations of each of the coordinates in the set $\{x_n\}$ as they are integrated over their infinite range means that the differences $\Delta x = x_{n+1} - x_n$ in the discretized action Eq. (34) do not formally to go to zero when the time interval $\Delta t \equiv \epsilon$ does as is required in the definition of the derivative (velocity) $\dot{x}(t) = \lim_{\Delta t\to 0} \Delta x/\Delta t$. The situation however is more subtle. The $\epsilon$ dependence of the first term in Eq. (34) indicates that for $|x_{n+1} - x_n|^2 \gg const\ \epsilon$ the integrand in Eq. (33) oscillates wildly giving negligible contribution. The relevant range is therefore $|\Delta x| \sim \sqrt{\epsilon}$. THIS MEANS THAT THE PATHS ARE CONTINUOUS BUT MOSTLY NON-DIFFERENTIABLE. EXPLAIN.

### 2.1.5 Time dependent Hamiltonian

Let us note that the path-integral representation (33) remains valid also for time-dependent potentials $V(x,t)$ with the corresponding value of the potential taken at each step. Thus follows from the form the time evolution operator (10) takes for time dependent $H_{op}(t)$

$$U(t_f, t_i) = \lim_{N\to\infty} \hat{T} \prod_{n=0}^{N-1} (1 - iH_{op}(t_n)\epsilon/\hbar) \quad , \quad \epsilon = \frac{t_f - t_i}{N} \tag{40}$$

with $t_0 = t_i$ and $t_n = t_i + n\epsilon$. The operator $\hat{T}$ is called time-ordering operator and its presence means that in the product the infinitesimal time evolution operators $(1 - iH_{op}(t_n)\epsilon/\hbar)$ (which do not usually commute) must act in the order of increasing times $t_n$, i.e. $t_{N-1} > t_{N-2} > ... > t_2 > t_0$. The above expression for $U(t_f, t_i)$ follows directly from the Schrödinger equation (7) for time dependent $H_{eq}(t)$ written in the form

$$\lim_{\epsilon\to 0} \ |\Psi(t+\epsilon)\rangle = (1 - iH_{op}(t)\epsilon/\hbar)|\Psi(t)\rangle \tag{41}$$

It is formally written using $\hat{T}$ as

$$U(t_f, t_i) = \hat{T} \exp\left[-\frac{i}{\hbar}\int_{t_i}^{t_f} dt\, H_{op}(t)\right] \tag{42}$$

and is called time ordered exponential.

For Hamiltonian Eq. (29) with time dependent $V(x,t)$ one can use the expression (40) and inserting complete sets of coordinate states

$$\int_{-\infty}^{\infty} |x_n\rangle\langle x_n| dx_n = 1 \quad , \quad n = 1, ..., N-1$$

as in Eq. (28) one can repeat all the steps leading to the expression (33) with $V(x,t)$ replacing $V(x)$.

### 2.1.6 Many dimensions

The above path integration formalism is straightforwardly generalized from one to any number of degrees of freedom as long as they are described by cartesian coordinates and the corresponding Hamiltonian has the same form as in Eq. (29) of a sum of quadratic kinetic energy terms with constant masses and a potential. As an example for a particle in 3 dimensions with the Hamiltonian

$$H_{op} = \frac{\mathbf{p}_{op}^2}{2m} + V(\mathbf{r}) \tag{43}$$

one finds

$$\begin{aligned} K(\mathbf{r}_f, t_f; \mathbf{r}_i, t_i) &= \lim_{\epsilon\to 0}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{3N/2} \int \prod_{n=1}^{N-1} d^3 r_n \\ &\quad \times \exp\left\{\frac{i}{\hbar}\sum_{n=1}^{N}\epsilon\left[\frac{m}{2}\left(\frac{\mathbf{r}_n - \mathbf{r}_{n-1}}{\epsilon}\right)^2 - V(\mathbf{r}_{n-1})\right]\right\} \to \\ &\quad \to \int D\mathbf{r}(t) \exp\left[(i/\hbar)\int_{t_i}^{t_f} dt L\left(\mathbf{r}(t), \dot{\mathbf{r}}(t)\right)\right] \end{aligned} \tag{44}$$

with fixed

$$\mathbf{r}_0 \to \mathbf{r}(t_i) = \mathbf{r}_i \ , \ \mathbf{r}_N \to \mathbf{r}(t_f) = \mathbf{r}_f$$

ADD DISCUSSION OF PATH INTEGRALS IN CARTESIAN VS NON CARTESIAN COORDINATES.

### 2.1.7 Phase space path integral

Let us step back to the basic relation (30) for infinitesimal propagator and transform it in a more general way

$$\lim_{\epsilon\to 0}\langle x_n|e^{-iH_{op}\epsilon/\hbar}|x_{n-1}\rangle = \langle x_n|1-i\epsilon H_{op}/\hbar + O(\epsilon^2)|x_{n-1}\rangle = \\ = \int dp_{n-1}\langle x_n|1-i\epsilon H_{op}/\hbar + O(\epsilon^2)|p_{n-1}\rangle\langle p_{n-1}|x_{n-1}\rangle \tag{45}$$

Using

$$\langle x_n|H_{op}|p_{n-1}\rangle = \langle x_n|\frac{p_{op}^2}{2m}+V(x_{op})|p_{n-1}\rangle = \left[\frac{p_{n-1}^2}{2m}+V(x_n)\right]\langle x_n|p_{n-1}\rangle \tag{46}$$

and denoting

$$H(p_{n-1},x_n) = \left[\frac{p_{n-1}^2}{2m}+V(x_n)\right] \tag{47}$$

we obtain

$$\lim_{\epsilon\to 0}\langle x_n|e^{-iH_{op}\epsilon/\hbar}|x_{n-1}\rangle = \tag{48}$$
$$= \int dp_{n-1}\langle x_n|p_{n-1}\rangle\langle p_{n-1}|x_{n-1}\rangle\left[1-i\epsilon H(p_{n-1},x_n)/\hbar + O(\epsilon^2)\right] = \\ = \int \frac{dp_{n-1}}{2\pi\hbar}e^{ip_{n-1}(x_n-x_{n-1})/\hbar}\left[1-i\epsilon H(p_{n-1},x_n)/\hbar + O(\epsilon^2)\right] = \\ = \int \frac{dp_{n-1}}{2\pi\hbar}\left[e^{ip_{n-1}(x_n-x_{n-1})/\hbar - i\epsilon H(p_{n-1},x_n)/\hbar} + O(\epsilon^2)\right]$$

Using this expression in Eq. (28) with q replaced by x and taking the limit $N\to\infty$, $\epsilon\to 0$ we now obtain

$$K(x_f,t_f;x_i,t_i) = \lim_{\epsilon\to 0}\int\prod_{n=1}^{N-1}dx_n\prod_{n=0}^{N-1}\frac{dp_n}{2\pi\hbar}\exp[\frac{i}{\hbar}S(x_1,...,x_{N-1};p_0,....p_{N-1})] \tag{49}$$

with

$$S(x_1,...,x_{N-1};p_0,....p_{N-1}) = \sum_{n=1}^{N}\epsilon\left[p_{n-1}\frac{x_n-x_{n-1}}{\epsilon}-H(p_{n-1},x_n)\right] \tag{50}$$

and fixed $x_0 = x_i$, $x_N = x_f$.

This expression for $S(x_1, ..., x_{N-1}; p_0, ....p_{N-1})$ is a discretized version of the functional in phase space

$$S[x(t), p(t)] = \int_{t_i}^{t_f} dt \left[ p(t) \frac{dx(t)}{dt} - H(p, x) \right] \tag{51}$$

with the boundary conditions $x(t_i) = x_i \ , \ x(t_f) = x_f$. It is the action in the Hamiltonian formulation of classical mechanics with $H(p, x)$ the classical Hamiltonian. With such action one uses the obvious symbolic notation of the Hamiltonian path integral of (49) as

$$K(x_f, t_f; x_i, t_i) = \int Dx(t) Dp(t) e^{i/\hbar S[x(t), p(t)]} \tag{52}$$

Let us notice that as Eq. (49) shows the integration measure $Dx(t)Dp(t)$ contains one extra integration over $dp_0$ and is divided by the N "phase space quantum unit cell" factors $2\pi\hbar$ for the present one dimensional system. For M dimension these become $(2\pi\hbar)^M$.

DISCUSS THE "DISCONTINUOUS NATURE" OF THE PATHS IN PHASE SPACE (SINCE NO DERIVATIVES $dp/dt$ UNLIKE IN COORDINATES).

DISCUSS DIFFERENT POSSIBILITIES OF "INSERTING" THE p-INTEGRATION IN EQ. (45) AND RESULTING AMBIGUITIES.

In our derivation of the path integral expressions Eqs. (33,49) we have explicitly used the special form of the Hamiltonian $H_{op}$, Eq. (29) as a sum of the separate momentum and coordinate dependent terms. Although such Hamiltonians are most common there are however physical systems with Hamiltonians which contain terms depending on both coordinate and momentum operators. Probably the simplest is the Hamiltonian of a charged particle in an external magnetic field

$$H_{op} = \frac{1}{2m} (\mathbf{p}_{op} - q\mathbf{A}(\mathbf{r}))^2 \tag{53}$$

We will deal with such a physical system in detail in appropriate Chapter of this notes. At the moment let us ask how to construct path integral formalism for such Hamiltonians.

To make this discussion reasonably general let us assume that we deal with a physical system described by cartesian coordinates $\mathbf{r}$ and Hermitian Hamiltonian $H_{op}$ given by a general function of the corresponding momentum and coordinate operators

$$H_{op} = H(\mathbf{p}_{op}, \mathbf{r}_{op}) \tag{54}$$

DERIVE. DISCUSS.

### 2.1.8 Comparing the canonical and path integral approaches

### 2.1.9 Convergence and related issues

## 2.2 Example - harmonic oscillator

Let us calculate the path integral Eq. (38) for a simple and very useful example - harmonic oscillator, i.e. for the potential in Eq. (29) given by

$$V(x) = \frac{1}{2}m\omega^2 x^2 \tag{55}$$

### 2.2.1 Expanding around the classical solution

The action integral for such a potential is

$$S_{h.o.}[(x(t)] = \int_{t_i}^{t_f} dt \left(\frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2\right) \tag{56}$$

To calculate the path integral Eq. (38) with such action we use the change of variables

$$x(t) = x_{cl}(t) + y(t) \tag{57}$$

where $x_{cl}(t)$ is the classical path. It obeys the standard harmonic oscillator equation of motion with the boundary conditions

$$\ddot{x}_{cl} + \omega^2 x_{cl} = 0 \quad \text{with} \quad x_{cl}(t_i) = x_i \ , \ x_{cl}(t_f) = x_f \tag{58}$$

so the shifted variables $y(t)$ obey

$$y(t_i) = y(t_f) = 0 \tag{59}$$

Under this transformation the path integral differential volume Eq. (39) will not change $Dx(t) = Dy(t)$ since for every element $dx_n$ of the path differential only a shift

$$x_n \equiv x(t_n) = x_{cl}(t_n) + y(t_n) \equiv x_{cl}(t_n) + y_n$$

takes place so $dx_n = dy_n$.

To simplify the substitution of the new variables it is useful to rewrite the action Eq. (56) integrating by parts its first kinetic energy term

$$S_{h.o.}[(x(t)] = \frac{1}{2}m[x_f\dot{x}(t_f) - x_i\dot{x}(t_i)] - \frac{m}{2}\int_{t_i}^{t_f}[x(\ddot{x} + \omega^2 x)]dt \tag{60}$$

In the new variables $S[x(t)]$ is a sum

$$S[x(t)] = S[x_{cl}(t) + y(t)] = S_{cl}^{h.o.} + \frac{1}{2}\delta^2 S[y(t)] \tag{61}$$

with

$$S_{cl}^{h.o.} \equiv S[x_{cl}(t)] = \frac{1}{2}m[x_f \dot{x}_{cl}(t_f) - x_i \dot{x}_{cl}(t_i)] \tag{62}$$

and the functional of the second variation $\delta^2 S$ around the classical path due to $y(t)$

$$\begin{aligned} \delta^2 S[y(t)] \;\equiv\; & \int_{t_i}^{t_f} dt \int_{t_i}^{t_f} dt' \frac{\delta^2 S}{\delta x(t)\delta x(t')}\bigg|_{x(t)=x_{cl}(t)} y(t)y(t') = \\ & = \int_{t_i}^{t_f} dt\, y(t)(-m\frac{d^2}{dt^2} - m\omega^2)y(t) \end{aligned} \tag{63}$$

The above (functional) Taylor expansion of the harmonic oscillator action stops after the second term since the action is quadratic and the first variation vanishes since we are expanding around the classical path.

Using Eq. (61) the propagator path integral for harmonic oscillator is written

$$K_{h.o.}(x_f, t_f; x_i, t_i) = F_{h.o.}(t_f, t_i) e^{iS_{cl}^{h.o.}/\hbar} \tag{64}$$

where the *h.o.* stands for "harmonic oscillator" and the reduced propagator $F_{h.o.}(t_f, t_i)$ is given by the path integral over the path variations $y(t)$ with respect to the classical path

$$F_{h.o.}(t_f, t_i) = \int_{y(t_i)=0}^{y(t_f)=0} Dy(t) e^{i\delta^2 S[y(t)]/2\hbar} \quad , \quad Dy(t) \equiv \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2} \prod_{n=1}^{N-1} dy_n \tag{65}$$

The classical action $S_{cl}$ in Eq. (64) is easy to calculate using the classical solution of Eq. (58) which is conveniently written as

$$x_{cl}(t) = \frac{1}{\sin\omega T}\left\{x_i \sin[\omega(t_f - t)] + x_f \sin[\omega(t - t_i)]\right\} \;\; ; \;\; T = t_f - t_i \tag{66}$$

This gives when inserted in Eq. (62)

$$S_{cl}^{h.o.} = \frac{m\omega}{2\sin\omega T}\left[(x_i^2 + x_f^2)\cos\omega T - 2x_i x_f\right] \tag{67}$$

So we are left with calculating $F_{h.o.}(t_f, t_i)$.

### 2.2.2 "Doing" the (simplest) Gaussian path integral

Let us begin by noticing that the form of $\delta^2 S[y(t)]$ in Eq. (65) and the boundary conditions of $y(t)$ indicate that $F_{h.o.}(t_f, t_i)$ is independent of $x_i$ and $x_f$. In addition due to the time translational invariance it can only depend on the difference $T = t_f - t_i$. We next observe that $\delta^2 S[y(t)]$ can be viewed as an expectation value of the operator

$$\Lambda \equiv -m\frac{d^2}{dt^2} - m\omega^2 \tag{68}$$

acting in the space of functions $y(t)$ with $t_i \leq t \leq t_f$ and the boundary conditions Eq. (59). Using Dirac notations

$$\delta^2 S[y(t)] = \langle y|\Lambda|y\rangle \tag{69}$$

Following the example of evaluating multidimensional Gauss integrals, cf., Appendix 5.2.2 let us make a change of variables in $\delta^2 S[y(t)]$ by expanding

$$y(t) = \sum_n a_n u_n(t) \tag{70}$$

and choosing $u_n(t)$ as the eigenfunctions of $\Lambda$

$$\Lambda u_n(t) = \lambda_n u_n(t) \tag{71}$$

with the boundary conditions Eq. (59). One easily finds

$$u_n(t) = \sqrt{\frac{2}{T}} \sin\left[\frac{\pi n}{T}(t - t_i)\right] \quad , \quad \lambda_n = \frac{m\pi^2 n^2}{T^2} - m\omega^2 \quad , \quad n = 1, 2, ... \tag{72}$$

As eigenfunctions of the Hermitian operator $\Lambda$ or in alternative terminology as solutions of the classical Sturm–Liouville problem the functions $u_n(t)$ form a complete orthogonal set with normalization constant chosen to make it normalized

$$\int_{t_i}^{t_f} u_n(t) u_m(t) dt = \delta_{nm} \tag{73}$$

Inserting Eq. (70) in (69) and using Eq. (71) the second variation is written

$$\delta^2 S = \sum_n \lambda_n a_n^2 \tag{74}$$

as a sum of independent terms in the new variables.

We now want to transform the path integral Eq. (65) to the new variables. In that the set $\{u_n(t)\}$ in the transformation (70) is the analogue of the matrix of the transformation from the variables $y_m \equiv y(t_m)$ to $a_n$'s. In Appendix 5.3 we discuss the Jacobian of this transformation and show that it is a constant independent of the physical parameters of the problem. We shall combine it with the normalization factor in the path differential in Eq. (65), denote the result as $J_N$ and write using Eq. (74)

$$F_{h.o.}(t_f, t_i) = \lim_{N\to\infty} J_N \int \prod_{n=1}^{N} da_n \; e^{(i/2\hbar)\sum_n \lambda_n a_n^2} = \lim_{N\to\infty} \frac{J'_N}{\sqrt{\prod_{n=1}^{N} \lambda_n}} \tag{75}$$

where we absorbed the product of $\sqrt{2\pi\hbar i}$'s in the prefactor $J'_N$. We determine this factor by using its independence of the oscillator $\omega$, considering the limit of $\omega \to 0$, i.e. the free particle and comparing with the known free particle expression (25). This gives

$$F_{h.o.}(t_f, t_i) = F_{free\ particle}(t_f, t_i) \times \lim_{N\to\infty} \sqrt{\frac{\prod_{n=1}^{N} \lambda_n^{(0)}}{\prod_{n=1}^{N} \lambda_n}} \tag{76}$$

where $\lambda_n^{(0)}$ denote the $\omega \to 0$ limit of the expression (72) for $\lambda_n$. Using this expression together with Eq. (25) and the Euler product representation

$$\frac{\sin x}{x} = \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{\pi^2 n^2}\right)$$

we obtain

$$F_{h.o.}(t_f, t_i) = \sqrt{\frac{m}{2\pi i\hbar T}} \times \lim_{N\to\infty} \left[\prod_{n=1}^{N} (1 - \frac{\omega^2 T^2}{\pi^2 n^2})\right]^{-1/2} = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}} \tag{77}$$

DISCUSS THE DIVERGENCES AND THE PHASE OF $F_{h.o.}(t_f, t_i)$, cf., Fig. 2

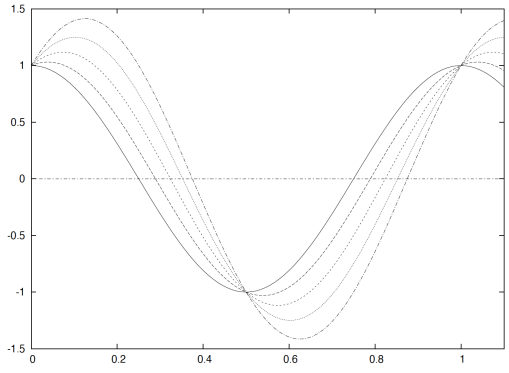


Figure 2: Classical trajectories of a harmonic oscillator. Trajectories which start at some point $x_i$ all meat again at $-x_i$ after half period $\tau = \pi/\omega$, independently of the initial velocity. After $N$ half periods the meeting point is at $(-1)^N x_i$

## 2.3 Perturbation expansion

The path integral formulation is ideally suited to develop perturbation theory approach when the potential or a physically important part of it can be treated as a small perturbation. Let us demonstrate this for simplicity again discussing the one dimensional case with the Hamiltonian given by Eq. (29) and the corresponding action Eq. (35) and the path integral Eq. (38). Expanding the exponential of the action in powers of the potential and denoting

$$L_0(\dot{x}(t)) = \frac{m}{2}\left(\frac{dx}{dt}\right)^2 \tag{78}$$

we obtain

$$\begin{aligned} K(x_f,t_f;x_i,t_i) &= \int Dx(t)\exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f} L_0(\dot{x}(t))dt\right]\sum_{j=0}^{\infty}\frac{1}{j!}\left[-\frac{i}{\hbar}\int_{t_i}^{t_f} V(x(\tau))\,d\tau\right]^j = \\ &= \sum_{j=0}^{\infty}\left(-\frac{i}{\hbar}\right)^j K_j(x_f,t_f;x_i,t_i) \end{aligned} \tag{79}$$

with

$$\begin{aligned} &K_j(x_f,t_f;x_i,t_i) = \\ &= \frac{1}{j!}\int_{t_i}^{t_f} d\tau_1 ... \int_{t_i}^{t_f} d\tau_j \int Dx(t) V(x(\tau_1))...V(x(\tau_j)\exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f} L_0(\dot{x}(t))dt\right] \end{aligned} \tag{80}$$

The $j = 0$ term of the above expression

$$K_0(x_f, t_f; x_i, t_i) = \int Dx(t) \exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f} L_0(\dot{x}(t))dt\right] \tag{81}$$

is just the free particle propagator, cf., Eq. (25). Let us consider the $j = 1$ term. Using the path integral property similar to a matrix product, cf., Eq. (28),

$$\int_{x(t_i)=x_i}^{x(t_f)=x_f} Dx(t)e^{(i/\hbar)S[x(t)]} = \int_{-\infty}^{\infty} d\xi \int_{x(t_i)=x_i}^{x(\tau)=\xi} Dx(t)e^{(i/\hbar)S[x(t)]} \int_{x(\tau)=\xi}^{x(t_f)=x_f} Dx(t)e^{(i/\hbar)S[x(t)]} \tag{82}$$

one can transform the expression for $j = 1$ term as

$$K_1(x_f, t_f; x_i, t_i) = \int_{t_i}^{t_f} d\tau_1 \int_{-\infty}^{\infty} d\xi_1 K_0(x_f, t_f; \xi_1, \tau_1)V(\xi_1)K_0(\xi_1, \tau_1; x_i, t_i) \tag{83}$$

where we denoted $\xi_1 = x(\tau_1)$.

To understand how to generalize the above expression for the terms (80) with arbitrary $j$ it is instructive to consider the $j = 2$ case. It is not difficult to see that the $\tau_1 \leftrightarrow \tau_2$ symmetry of the integrand allows to write the double integral over the $t_i \le \tau_1, \tau_2 \le t_f$ square as twice the integral over the triangle

$$t_i \le \tau_1 \le \tau_2 \quad , \quad t_i \le \tau_2 \le t_f$$

with the result

$$\begin{aligned} K_2(x_f, t_f; x_i, t_i) \;\; = \;\; & \int_{t_i}^{t_f} d\tau_2 \int_{-\infty}^{\infty} d\xi_2 \int_{t_i}^{\tau_2} d\tau_1 \int_{-\infty}^{\infty} d\xi_1 K_0(x_f, t_f; \xi_2, \tau_2) \;\times \\ & \times V(\xi_2)K_0(\xi_2, \tau_2; \xi_1, t_1)V(\xi_1)K_0(\xi_1\tau_1; x_i, t_i) \end{aligned} \tag{84}$$

and notation $\xi_i = x(\tau_i)$. The essential feature of this expression is the time ordered product of free propagations "interrupted" by the interactions. Historically such expression derived within the path integral approach let Feynman to develop the graphic representation known as Feynman diagrams, cf. Fig. 3.

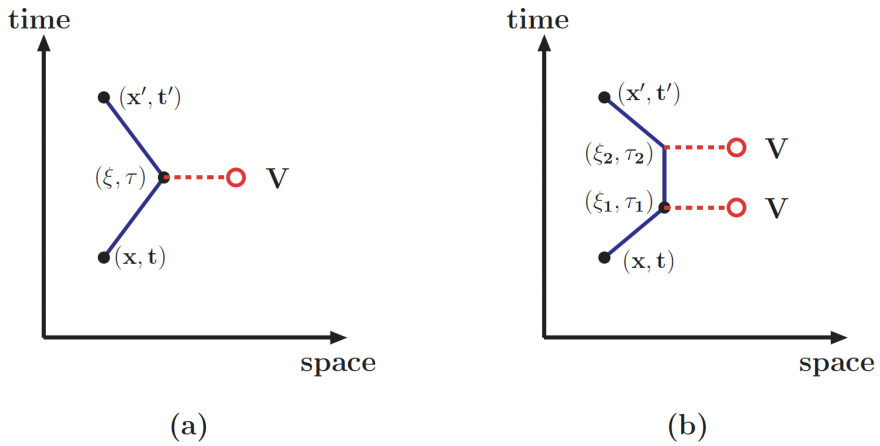


Figure 3: Feynman diagrams for the 1st and 2nd order perturbation theory of the propagator, Eqs. (83) and (84). The solid lines represent the free propagator between two space-time points, the dashed lines the interaction potential V. Intermediate points are to be integrated over

This $j = 2$ example helps to rewrite the general expression (80) in a time ordered way

$$K_j(x_f, t_f; x_i, t_i) = \tag{85}$$
$$= \int_{t_i}^{t_f} d\tau_j \int_{-\infty}^{\infty} d\xi_j \int_{t_i}^{\tau_j} d\tau_{(j-1)} \int_{-\infty}^{\infty} d\xi_{(j-1)} ... \int_{t_i}^{\tau_2} d\tau_1 \int_{-\infty}^{\infty} d\xi_1 K_0(x_f, t_f; \xi_j, \tau_j) V(\xi_j) \times$$
$$\times K_0(\xi_j, \tau_j; x_{j-1}, \tau_{j-1}) V(\xi_{(j-1)}) .... K_0(\xi_2, \tau_2; x_1, \tau_1) V(\xi_1) K_0(\xi_1, \tau_1; x_i, t_i)$$

Let us note that the above expression can be written as a recursion relation for the $K_j$ terms

$$K_j(x_f, t_f; x_i, t_i) = \int_{t_i}^{t_f} d\tau \int_{-\infty}^{\infty} d\xi K_0(x_f, t_f; \xi, \tau) V(\xi) K_{j-1}(\xi, \tau; x_i, t_i) \tag{86}$$

Using this one can write the expansion (79) as

$$\begin{aligned} K &= K_0 + \sum_{j=1}^{\infty} \left(-\frac{i}{\hbar}\right)^j K_j(x_f, t_f; x_i, t_i) = \\ &= K_0 + \sum_{j=1}^{\infty} \left(-\frac{i}{\hbar}\right)^j \int_{t_i}^{t_f} d\tau \int_{-\infty}^{\infty} d\xi K_0(x_f, t_f; \xi, \tau) V(\xi) K_{j-1}(\xi, \tau; x_i, t_i) = \\ &= K_0 - \frac{i}{\hbar} \int_{t_i}^{t_f} d\tau \int_{-\infty}^{\infty} d\xi K_0(x_f, t_f; \xi, \tau) V(\xi) \sum_{j=1}^{\infty} \left(-\frac{i}{\hbar}\right)^{(j-1)} K_{j-1}(\xi, \tau; x_i, t_i) \end{aligned} \tag{87}$$

Changing the summation index $j = j' + 1$ one obtains an integral equation for the propagator

$$K(x_f, t_f; x_i, t_i) = K_0(x_f, t_f; x_i, t_i) - \frac{i}{\hbar} \int_{t_i}^{t_f} d\tau \int_{-\infty}^{\infty} d\xi K_0(x_f, t_f; \xi, \tau) V(\xi) K(\xi, \tau; x_i, t_i) \tag{88}$$

DISCUSS. EXPLAIN THESE RELATIONS IN OPERATOR FORM FOR THE TIME EVOLUTION OPERATOR $U(t_f, t_i)$. GO TO THE E-DEPENDENT GREEN's FUNCTION AND DERIVE THE LIPPMANN-SCHWINGER EQUATION.

## 2.4 Semiclassical limit

Compared to the conventional Schrödinger picture the path integral approach offers a very different view on the quantum mechanical description of the dynamics of physical systems. In this Section we will discuss how the semiclassical limit is obtained in this approach. We will compare the results with the semiclassical limit of the Schrödinger equation.

### 2.4.1 "Deriving" the Hamilton action principle

In the path integral expressions for the propagator, e.g. Eq. (44) each path has equal probability and seems equally important. The difference of course is in the phase $S[path]/\hbar$ and the fact that different paths interfere with one another in their contribution to the total probability of propagation between given initial and final points. The classical limit of this interference occurs when the parameters of the physical system, i.e. masses, parameters of the potential, are such that for small changes of a path $\Delta[path]$ the corresponding change $\Delta S$ of the action is much larger than the Planck constant $\hbar$.

$$\Delta S/\hbar \gg 1 \tag{89}$$

These large changes of the phases of the path amplitudes mean that on the average they interfere destructively with negligible contribution to the total propagation probability. The situation is different for a classical path for which the action is stationary

$$\delta S = 0 \tag{90}$$

The paths near such path will have small phase differences and on average interfere constructively. In the classical limit they will produce dominant contribution to the total propagation probability. In other words in the classical limit physical systems are described with high accuracy as propagating along paths which satisfy Eq. (90) which is the familiar Hamilton Action Principle from which the Euler-Lagrange equations of classical mechanics are derived.

### 2.4.2 Semiclassical propagator. Gaussian fluctuations

Classical path solutions of Eq. (90) obviously define the stationary points of the integrand in the path integral expression for the propagator. We will now use the stationary phase method as reviewed in Appendix 5.2 to obtain the corresponding semiclassical approximation to the path integral. We will work for simplicity with the path integral Eq. (38) with the action Eq. (35) of a physical system moving in just one dimension. We will then generalize our results to many dimensional cases.

Let us consider a classical path $x_{cl}(t)$ satisfying the Euler-Lagrange equation which follows from Eq. (90) and the expression (35) for the action

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x} \quad \rightarrow \quad m\frac{d^2 x_{cl}}{dt^2} = -\frac{\partial U(x_{cl})}{\partial x} \tag{91}$$

and the propagator end points defined boundary conditions

$$x_{cl}(t_i) = x_i \ , \ \ x_{cl}(t_f) = x_f \tag{92}$$

We assume that a) such path exists and b) that there is just one such path. We will discuss below that this is not always the situation due to the fact that the boundary rather than initial conditions are imposed. We will then describe how to extend our present treatment of one path to such cases.

As in the harmonic oscillator case let us change the path integration variables

$$x(t) = x_{cl}(t) + y(t) \tag{93}$$

with the boundary conditions for the shifted $y(t)$

$$y(t_i) = y(t_f) = 0 \tag{94}$$

With this shift we can write using similar notations as in the harmonic oscillator Eq. (64)

$$K(x_f,t_f;x_i,t_i)=e^{(i/\hbar)S[x_{cl}(t)]}\int Dx(t)e^{(i/\hbar)\}S[x(t)]-S[x_{cl}(t)]\}}\equiv F(x_f,t_f;x_i,t_i)e^{(i/\hbar)S[x_{cl}(t)]} \tag{95}$$

then expand

$$S[x(t)]=S[x_{cl}(t)]+(1/2!)\delta^2S[y(t)]+(1/3!)\delta^3S[y(t)]+\dots\,,$$

and following the standard practice of the stationary phase method approximate the deviations of $S[x(t)]$ from the classical path value by keeping the first non vanishing term

$$F(x_f,t_f;x_i,t_i)\approx\int Dy(t)e^{(i/2\hbar)\delta^2S[y(t)]} \tag{96}$$

The term $\delta^2S[y(t)]$ is the second variation in terms of the shifted $y(t)$ paths as we have already encountered in the harmonic oscillator case, Eq. (63). In the present more general case we obtain

$$\frac{1}{2}\delta^2S[y(t)]=\int_{t_i}^{t_f}dt\,\left[\frac{m}{2}\dot{y}^2-\frac{1}{2}U''(x_{cl}(t))y^2\right] \tag{97}$$

One sees that $(1/2)\delta^2S[y(t)]$ can be viewed as an action of a harmonic oscillator with a time-dependent oscillator constant

$$\omega^2(t)=\frac{1}{m}U''[x_{cl}(t)] \tag{98}$$

and the boundary conditions Eq. (94).

Let us also remark that unlike in the harmonic oscillator case with the constant $\omega$ the path integral in Eq. (96) will in general retain the dependence on the initial and final coordinates via the dependence of $U''[x_{cl}(t)]$ on the classical path. We have made this dependence explicit in the notation $F(x_f,t_f;x_i,t_i)$ for this integral.

### 2.4.3 Heuristic derivation - one dimension

The following simple arguments are useful in discussing the semiclassical propagator as described by Eqs. (95) and (96). Classically the propagation from $x_i$ at $t_i$ to $x_f$ at $t_f$ requires a defined initial momentum $p_i\equiv p(t_i)$. Changing $x_f$ to $x_f+dx_f$ means changing $p_i\to p_i+dp_i$. Since quantum mechanically for a fixed $x_i$ the probability of

$p_i$ is uniformly distributed as $w(p_i)dp_i = dp_i/(2\pi\hbar)$ the probability of a propagation into the interval $x_f \leq x \leq x_f + dx_f$ at $t_f$ is

$$|K(x_f, t_f; x_i, t_i)|^2 dx_f = \frac{dp_i}{2\pi\hbar} = \frac{1}{2\pi\hbar}\frac{dx_f}{|dx_f/dp_i|} \tag{99}$$

This gives for the absolute value of the semiclassical amplitude in Eq. (95)

$$|F(x_f, t_f; x_i, t_i)| = \frac{1}{\sqrt{2\pi\hbar|dx_f/dp_i|}} \tag{100}$$

One can use the energy conservation to obtain a more explicit expression for the $dx_f/dp_i$ with the result (cf., Appendix)

$$\frac{dx_f}{dp_i} = p_(x_i)p_(x_f)\int_{x_i}^{x_f}\frac{dx}{p^3(x)} \quad \text{with} \quad p(x) = \sqrt{2m(E_{cl}(T) - V(x))} \tag{101}$$

with the energy $E_{cl}(T)$ a function of $x_i, t_i, x_f, t_f$ given by the implicit relation

$$T \equiv t_f - t_i = \int_{x_i}^{x_f} dx\sqrt{\frac{m}{2(E_{cl}(T) - V(x))}} \tag{102}$$

The corresponding action is

$$S_{cl}(x_i, x_f; T) = \int_{x_i}^{x_f} p(x)dx - E_{cl}(T)T \tag{103}$$

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MOVE THIS PART TO THE APPENDIX

$$E = \frac{p_f^2}{2m} + V(x_f) = \frac{p_i^2}{2m} + V(x_i) \quad , \quad \left(\frac{2}{m}\left(E - V(x)\right)\right)^{1/2} = \frac{dx}{dt}$$

Differentiating Eq. (102) with respect to $p_i$ and using

$$\frac{\partial E}{\partial p_i} = \frac{p_i}{m}$$

obtain

$$0 = \sqrt{\frac{m}{2(E - V(x_f))}}\frac{dx_f}{dp_i} - \frac{p_i}{m}\int_{x_i}^{x_f} dx\frac{\sqrt{m}}{(2(E - V(x)))^{3/2}}$$

which gives Eq. (101). The corresponding action is

$$S_{cl} = \int_{t_i}^{t_f} (\frac{m\dot{x}^2}{2} - V(x))dt = \int_{t_i}^{t_f} m\dot{x}^2 dt - E(t_f - t_i) \tag{104}$$

giving the result Eq. (103)

NOTE - $p(x)$ may have two branches for classical trajectories with turning points. THIS POSSIBILITY NOT ACCOUNTED YET IN THE ABOVE EXPRESSIONS

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### 2.4.4 The Van Vleck determinant. Many dimensions

Let us recall that the classical action $S_{cl}$ is a function of the initial and final coordinates and times

$$S_{cl} = S_{cl}(x_i, t_i; x_f, t_f) \tag{105}$$

Its derivatives obey simple relations

$$p_i = -\frac{\partial S_{cl}(x_i, t_i; x_f, t_f)}{\partial x_i} \quad , \quad p_f = \frac{\partial S_{cl}(x_i, t_i; x_f, t_f)}{\partial x_f} \tag{106}$$

which are simple to derive using the familiar expression for the variation of $S$, Eq. (35)

$$\delta S = \frac{\partial L}{\partial \dot{x}(t)} \delta x(t) \Big|_{t_i}^{t_f} - \int_{t_i}^{t_f} dt \left( \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} \right) \delta x(t) \tag{107}$$

Since $\partial L / \partial \dot{x}(t) = p(t)$ and for the classical path the integrand vanishes one obtains the relations (106). Using the first of this relations one can express

$$|F(x_f, t_f; x_i, t_i)| = \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\left| \frac{\partial S_{cl}}{\partial x_i \partial x_f} \right|} \tag{108}$$

It is straightforward to generalize the above discussion to M (cartesian) dimensions with $x$ and $p$ denoting $x = (x_1, ..., x_M)$ and $p = (p_1, ..., p_M)$ and using the notation $x(t_i), p(t_i)$ for $x_i, p_i$ and $x(t_f), p(t_f)$ for $x_f, p_f$ to avoid double indexing.

The expression (99) becomes

$$|K(x(t_f), t_f; x(t_i), t_i)|^2 \prod_{m=1}^{M} dx_m(t_f) = \prod_{n=1}^{M} \frac{dp_n(t_i)}{2\pi\hbar} \tag{109}$$

Using the Jacobian

$$\prod_{n=1}^{M} dx_m(t_f) = \det\left[\frac{\partial x_m(t_f)}{\partial p_n(t_i)}\right] \prod_{n=1}^{M} dp_n(t_i) \tag{110}$$

and the $M$ dimensional version of Eq. (95 we obtain

$$\begin{aligned} |K(x(t_f),t_f;x(t_i),t_i)| &= |F(x(t_f),t_f;x(t_i),t_i)| = \\ &= \frac{1}{(2\pi\hbar)^{M/2}\sqrt{|\det\left[\partial x_m(t_f)/\partial p_n(t_i)\right]|}} \end{aligned} \tag{111}$$

The $M$ dimensional version of the relations (106) allows the write this expression as

$$|F(x(t_f),t_f;x(t_i),t_i)| = \frac{1}{(2\pi\hbar)^{M/2}}\sqrt{\left|\det\left[\frac{\partial^2 S_{cl}}{\partial x_m(t_i)\partial x_n(t_f)}\right]\right|} \tag{112}$$

The determinant here is historically called the Van Vleck determinant, Ref. [7][2]. It can be shown, cf., Ref. [8] that the above expression is consistent with the unitarity of the semiclassical propagator. We will extend our discussion of this expression in the sections below.

### 2.4.5 Calculating the integral

We will now rederive/verify the expressions which were obtained in the previous section using simple heuristic arguments. We will do this by explicit evaluation of the Gaussian integral (96).

a) Determining $|F(x_f,t_f;x_i,t_i)|$

Our discussion will begin by following closely what was done in the harmonic oscillator case, Eq. (65). Using integration by parts the second variation (97) of the action in (96) can be written as

$$\delta^2 S[y(t)] = \int_{t_i}^{t_f} dt\, y(t)\Lambda y(t) \quad \text{with} \quad \Lambda = -m\frac{d^2}{dt^2} - \frac{\partial^2 U(x_{cl}(t))}{\partial x^2} \tag{113}$$

[2]In the literature one also finds this expression termed Van Vleck-Morette determinant or Van Vleck-Pauli-Morette determinant

As in Eq. (69) the expression for $\delta^2 S$ is an expectation value of the operator $\Lambda$ which is a generalized version of the simple harmonic oscillator case, Eq. (69). Repeating the steps there we make a change of variables in the above expression by expanding $y(t)$ as in Eq. (70) with $u_n(t)$ as the eigenfunctions of the present $\Lambda$ operator

$$\left[-m\frac{d^2}{dt^2} - \frac{\partial^2 U(x_{cl}(t))}{\partial x^2}\right] u_n(t) = \lambda_n u_n(t) \ \ , \ \ u_n(t_i) = u_n(t_f) = 0 \tag{114}$$

The rest of the formal steps to evaluate the Gaussian integral in Eq. (95) are identical to those in Sec. 2.2.2 with the final result given by the formally similar expression to Eq. (76)

$$F(x_f, t_f; x_i, t_i) = F_{free\ particle}(t_f, t_i) \times \lim_{N\to\infty} \sqrt{\frac{\prod_{n=1}^{N} \lambda_n^{(0)}}{\prod_{n=1}^{N} \lambda_n}} \tag{115}$$

The analogy with harmonic oscillator stops here however since in the present, general potential case one does not have explicit expressions for the eigenvalues $\lambda_n$ entering the denominator of Eq. (115). The formal reason is fairly clear - the second variation operator $\Lambda$ in Eq. (113) does not have constant coefficients as in Eq. (68). Rather it depends on time via the potential $U(x)$ and the classical path $x_{cl}(t)$ which are different for different physical systems and different initial and final conditions even for the same system.

One can avoid dealing with the products of eigenvalues in Eq. (115) by calculating the determinant of a discretized version of the $\Lambda$ operator. This was first done in Ref. [11] and is reviewed in e.g. Ref. [5],[12]. We will follow a different route based on the theorem proved in Ref. [13] the use of which for path integrals was presented in Ref. [14].

Consider the following initial value problem based on the operator $\Lambda$ in Eq. (113)

$$\Lambda\eta(t) \equiv \left[-m\frac{d^2}{dt^2} - \frac{\partial^2 U(x_{cl}(t))}{\partial x^2}\right] \eta(t) = 0 \tag{116}$$
$$\text{with initial conditions } \eta(t_i) = 0 \ , \ \dot{\eta}(t_i) = 1$$

and the same problem with $\Lambda$ replaced by $\Lambda_0 = -md^2/dt^2$. The solution of the latter we denote $\eta_0(t)$. This is easily found as

$$\eta_0(t) = (t - t_i) \tag{117}$$

It was proved in Ref. [13] that the ratio of the infinite products in Eq. (115) can be expressed in terms of the ratio of the values of these solutions at the final propagation

time $t_f$.

$$\lim_{N\to\infty}\left|\frac{\prod_{n=1}^{N}\lambda_n^{(0)}}{\prod_{n=1}^{N}\lambda_n}\right| = \left|\frac{\eta_0(t_f)}{\eta(t_f)}\right| \tag{118}$$

Before proceeding to use this relation to obtain a final expression for $|F(x(t_f),t_f;x(t_i),t_i)|$ let us examine the physical meaning of the solution $\eta(t)$ defined in (116). Unlike its "free" partner $\eta_0(t)$ this solution's general analytic expression can not be determined for an arbitrary potential $U(x)$. However it has a simple relation to the properties of the classical path $x_{cl}(t)$ with respect to which $\Lambda$ is defined. Let us show this.

As was discussed above, following Eq. (91) the classical path around which we expand the path integral is defined by the boundary conditions (2.3) at $t = t_i$ and $t = t_f$ contrary to the common practice of specifying the initial conditions at $t = t_i$. This feature is typical of the semiclassical theory and is discussed at length in Ref. [8]. However, once the classical path is found, the initial velocities are specified $\dot{x}_{cl}(t_i)$. Let us consider how the classical path changes under an infinitesimal change of the initial velocity with fixed initial coordinate i.e. the derivative $\partial x_{cl}(t)/\partial\dot{x}_{cl}(t_i)$ under the condition $x_{cl}(t_i) = x_i$. It is then straightforward to show by differentiating Eq. (91) with respect to $\dot{x}_{cl}(t_i)$ that the solution of the initial value problem Eq. (116) is equal to this derivative

$$\eta(t) = \partial x_{cl}(t)/\partial\dot{x}_{cl}(t_i)\big|_{x_{cl}(t_i)=x_i} \tag{119}$$

TALK ABOUT THE MEANING OF THIS EXPRESSION (JACOBI FIELD).

Using the solution (117) for $\eta_0(t)$ and the expression

$$F_{free\ particle}(t_f,t_i) = \sqrt{\frac{m}{2\pi i\hbar(t_f-t_i)}} \tag{120}$$

cf., Eq. (25), we arrive at the result (100) which we obtained earlier using less rigorous arguments. The generalization to $M$ dimensional system and most general Lagrangians can be fairly straightforwardly done, cf., Ref. [14] leading to the result Eq. (111). The $M$ dimensional version of Eq. (116) is known as Jacobi equations in variational calculus or as Poincare equations in stability theory.

b) Determining the phase of $F(x_f,t_f;x_i,t_i)$.

Let us examine the right-hand side of the expression (115). The free particle eigenvalues in this expression are all positive

$$\lambda_n^{(0)} = \frac{m\pi^2n^2}{T}\ \ ,\ \ T = t_f - t_i$$

cf., the $\omega \to 0$ limit of Eq. (72). Hence apart from the trivial factor $\sqrt{i}$ in the denominator of $F_{free\ particle}$, Eq. (120), the phase of $F(x_f, t_f; x_i, t_i)$ is given from (115) by $(-\nu\pi/2)$, where $\nu$ is the number of negative eigenvalues of the operator $\Lambda$ in the boundary problem (114).

The problem of determining $\nu$ has been extensively studied by Morse [9]. In analogy with the theory of quadratic forms in finite dimensional spaces, the number $\nu$ of the negative eigenvalues in this problem is called the index of the classical path $x_{cl}(t, x_i, x_f)$ on which the quadratic functional $\delta^2 S$, Eq. ( 113) is defined. The useful concept of focal or conjugate point is then introduced. The point $x_{cl}(\tau)$ on the classical path is a focal (conjugate) point relative to $x_i = x_{cl}(t_i)$ if Eq. (116) has a nonzero solution which vanishes at $t = \tau$. TALK ABOUT THE PHYSICAL MEANING OF SUCH POINTS. REFER TO THE EXAMPLE OF $1/x^2$ POTENTIAL ILLUSTRATING SUCH POINTS AND THEIR RELATION TO AN ENVELOPE OF CLASSICAL PATHS ALL PASSING THROUGH $x_i$ at $t = t_i$ AND CONTAINING THE PATH $x_{cl}(t, x_i, x_f)$. SUCH ENVELOPE SURFACE IS OFTEN REFERRED TO AS THE FOCAL SURFACE OR THE CAUSTIC. THIS IS BY ANSLOGY WITH GEOMETRICAL OPTICS (FIND A GOOD SIMPLE REFERENCE TO CAUSTICS IN MECHANICS AND OPTICS)

The main result of the Morse theory is that the index $\nu$ of the classical path is finite and is equal to the count of focal points on this path strictly between its end points. EXPLAIN QULITATIVELY THE PROOF OF THIS RESULT.

Thus the phase of the Gaussian path integral $F(x_f, t_f; x_i, t_i)$, Eq. (96) is thus given by $e^{-i\nu\pi/2}$ with $\nu$ the number of focal points along the classical trajectory with respect to which the integral is defined. This result is important when the contributions from several classical paths are considered and their relative phases affect the propagator through the interference phenomenon. In practice, in order to calculate $F(x_f, t_f; x_i, t_i)$ one has to solve Eq. (116). By following the time development of its solution $\eta(t)$ one obtains the phase of the propagator by counting the number of zeros along the path, whereas its absolute value is determined by $\eta(t_f)$.

c) Several degrees of freedom

EXPLAIN HOW THE ABOVE RESULTS OF THE PHASE OF $F(x_f, t_f; x_i, t_i)$ ARE GENERALIZED FOR $M$ DEGREES OF FREEDOM.

### 2.4.6 Least action or just stationary - how many classical trajectories? Caustics. Example $1/x^2$ potential

`http://www.scholarpedia.org/article/Principle_of_least_action#When_Action_is_a_Minimum`

# 3 Applying the semiclassical approximation

## 3.1 Energy quantization

Let us show how one can determine the energy eigenvalues of possible bound states of a physical system using the semiclassical approximation. Consider the energy dependent Green's function, Eq. (19) and calculate the trace of it

$$TrG(E) = \int_{-\infty}^{\infty} dx\, G(x,x;E) = \sum_m \frac{1}{E - E_m + i0} \tag{121}$$

Thus the position of the poles of $TrG(E)$ give the values of the eigenenerges of the problem.

Using the relation (15) of the time dependent Green's function to the propagator and the semiclassical approximation of the latter one has

$$\begin{aligned} G(x_f, x_i; E) &= \int_0^{\infty} \frac{dT}{2\pi\hbar} K(x_f, T, x_i; 0)\, e^{iET/\hbar} \approx \\ &\approx \int_0^{\infty} \frac{dT}{2\pi\hbar} F(x_f, T; x_i, 0) e^{i(S[x_{cl}(t)]+ET)/\hbar} \end{aligned} \tag{122}$$

Evaluating the time integral and the trace in Eq. (121) using the stationary phase approximation and summing the contributions of all the stationary points one can show (cf., Ref. [15], p.32, DERIVE THE DETAILS) that for a potential with a single minimum this method reproduces the WKB result that the energy levels are given by the Bohr-Sommerfeld quantization rule

$$\int_a^b p(x)dx = \int_a^b dx\sqrt{2m(E - V(x))} = \pi\hbar(n + 1/2) \tag{123}$$

where $a$ and $b$ are the classical turning point where $E = V(x)$.

EXPLAIN.

## 3.2 Tunneling via path integrals. Imaginary time

One of the conceptually novel applications of the path integrals is the semiclassical treatment of the quantum mechanical tunneling using classical solutions analytically continued to imaginary time. We will now present the basic elements of this approach in the context of one dimensional potential problems. Treatment of tunneling in such simple systems can be done using semiclassical WKB approximation to the Schrödinger equation. The advantage of the path integrals treatment is that it can be extended to tunneling in many dimensional, many body and field theoretical problems.

### 3.2.1 Simplest example - tunneling through potential barrier

Let us begin with a one dimensional potential barrier, cf., Fig. 4 and consider the propagation of a particle from a coordinate $x = x_i$ far left of the barrier to $x = x_f$ on its far right[3]. We will concentrate on the semiclassical approximation to the corresponding propagator as was discussed in Section 2.4.2 but we will look for two possible propagation condition - one with a given time $T = t_f - t_i$ and one with a given energy $E$.

To describe the semiclassical propagation with the given time one needs to find the classical trajectory connecting the points $x_i$ and $x_f$ in time $T = t_f - t_i$ and evaluate the corresponding semiclassical approximation of the propagator $K(x_f, t_f; x_i, t_i)$ as given by Eq. (95). For a one dimensional problem with time independent Hamiltonian the classical trajectory is easily found using the energy conservation as we demonstrated in Section 2.4.3 with the result

$$K(x_f, T; x_i, 0) = \left[2\pi\hbar\, p_(x_i)p_(x_f) \int_{x_i}^{x_f} \frac{dx}{p^3(x)}\right]^{-1/2} \times \times \exp\frac{i}{\hbar}\left[\int_{x_i}^{x_f} p(x)dx - E_{cl}(T)T\right] \tag{124}$$

where we used that for the time independent $V(x)$ the propagator $K$ depends on the difference $T = t_f - t_i$ rather than separately on $t_f$ and $t_i$.

[3] In this section we follow Ref. [16]

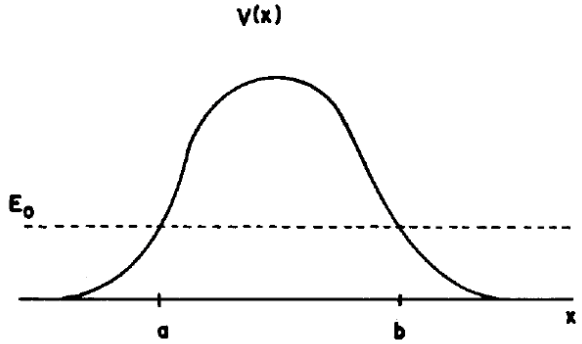


Figure 4: One dimensional potential barrier. For energies $E_0$ below the barrier top the classical turning points are defined by $V(a) = V(b) = E_0$.

It is important to understand that for any given $T$ there exists a classical trajectory with the energy implicitly given by the relation Eq. (102). Intuitively for very short $T$ the energy value will be high, i.e. much higher than the barrier while for very long times the energy will be very close to $V_{max}$ of the top of the barrier. Examining such trajectories for the fixed $x_i$ and different initial velocities $\dot{x}_i$'s leading to the given $x_f$ one can see that there are no focal points along the trajectories i.e. no points at which $\partial x_{cl}(t)/\partial \dot{x}_i$ vanishes, cf., Fig. 5. So according to our discussion in Sec. 2.4.5 there is no focal point phase in the above expression for $K(x_f, T; x_i, 0)$

Figure 5: Classical trajectories for the system with the barrier potential, cf., Fig. 4. The trajectories have different positive initial velocities $\dot{x}_i$ starting at a given initial $x_i$ to the left of the barrier and ending at $x_f$ to its right.

Let us now consider the energy dependent propagator given by Eq. (122) The explicit expressions for $F(x_f, T; x_i, 0)$ and $S[x_{cl}(t)]$ can be read off the equation (124). Following the semiclassical approach we use the stationary phase method to evaluate

the time integral in Eq. (122). The stationary phase condition is

$$E = -\frac{\partial S[x_{cl}(t)]}{\partial T} = E_{cl}(T) \tag{125}$$

where we used the known classical mechanics relation between the time derivative of the action calculated along a classical trajectory and the energy of this trajectory. The reader can find it useful to verify this relation by differentiating the explicit expression of the action in Eq. (124).

The above equation for $T$ has solutions only for energies above the barrier height as only for such energies there exist classical paths connecting points on the opposite sides of the barrier. Formally this is reflected in Eq. (102) which shows that $T$ becomes complex valued for $E < V_{max}$. This absence of the real valued stationary phase point for an integral with a rapidly oscillating semiclassical phase as we assume in Eq. (122) means that the integral is exponentially small. Following the rules of the stationary phase approximation method the value of the integral can be found using the saddle point (also known as steepest descent) generalization of this method. It uses complex valued solutions of the stationary point equation with integration contour deformed to pass through such points. We describe the details of this method in Appendix 5.2.3.

Let us examine the meaning of the complex valued solutions of Eq. (125) for $E < V_{max}$. We start with the observation that classical Newton equation to imaginary time $\tau = it$

$$m\frac{d^2x}{d\tau^2} = -m\frac{d^2x}{dt^2} = \frac{dV(x)}{dx} \quad \rightarrow \quad m\frac{d^2x}{d\tau^2} = \frac{dV(x)}{dx} \tag{126}$$

describe a classical particle moving in the inverted potential $-V(x)$. In the case of the barrier this becomes a potential well, cf., Fig. 6.

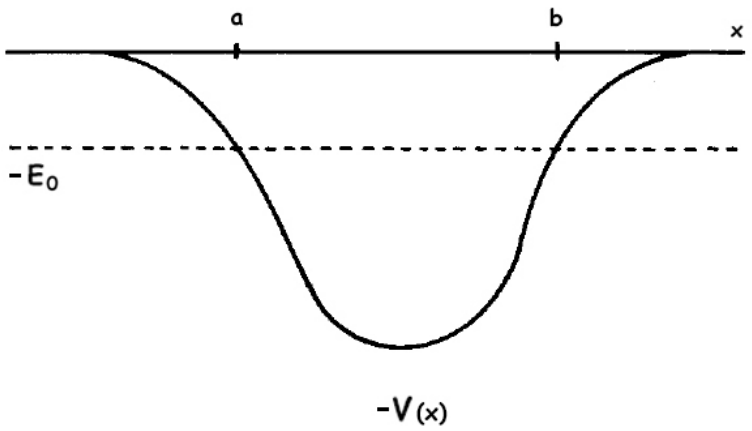


Figure 6: Inverted potential in which the particles moves in the imaginary time

Given such imaginary time propagation under the barrier the particle can travel from $a$ to $b$ in an infinite number of ways corresponding to an arbitrary number of loops bouncing in the inverted potential well from $b$ to $a$ and back to $b$ and exiting after an arbitrary number of such bounces. As is seen in Eq. (102) the simplest is just

$$T^{(0)} = \int_{x_i}^{a} dx \sqrt{\frac{m}{2(E-V(x))}} \quad - \quad i\int_{a}^{b} dx \sqrt{\frac{m}{2(V(x)-E)}} + \\ + \int_{b}^{x_f} dx \sqrt{\frac{m}{2(E-V(x))}} \tag{127}$$

The complex time $T^{(0)}$ describes the particle moving in real time from $x_f$ to the turning point $x = a$, switching to imaginary propagation time and "passing" through the sub-barrier region $a < x < b$ moving in the inverted $-V(x)$. When reaching the turning point at $x = b$ the propagation time switches back to real with particle moving from $b$ to $x_f$.

Trajectories bouncing n times inside the sub-barrier region obviously have

$$T^{(n)} \quad = \quad \int_{x_i}^{a} dx \sqrt{\frac{m}{2(E-V(x))}} - i(2n+1)\int_{a}^{b} dx \sqrt{\frac{m}{2(V(x)-E)}} + \\ + \int_{b}^{x_f} dx \sqrt{\frac{m}{2(E-V(x))}} \quad n = 0, 1, ... \tag{128}$$

One thus has a discrete infinity of complex valued solutions and must sum over the relevant ones evaluating the integral (122) by the saddle point method. Let us start with the $T^{(0)}$. As we show in Appendix (see also Refs. [16],[17]) the result is

$$G^{(0)}(x_f, x_i; E) \approx \frac{m\hbar}{2\pi} \frac{1}{\sqrt{p_(x_i) p_(x_f)}} \exp\left[\frac{i}{\hbar}\int_{x_i}^{x_f} p(x)dx\right] \tag{129}$$

with the complex valued phase factor

$$\int_{x_i}^{x_f} p(x)dx = \int_{x_i}^{a} p(x)dx + i\int_{a}^{b} p(x)dx + \int_{b}^{x_f} p(x)dx \tag{130}$$

reflecting the tunneling through the barrier.

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SHOULD BE MOVED TO APPENDIX.

Applying the saddle point approximation to the integral (122) for the saddle point $T^{(0)}$ gives

$$G^{(0)}(x_f, x_i; E) = F(x_f, T^{(0)}; x_i, 0)\left(\frac{2\pi\hbar}{i\gamma}\right)^{1/2} e^{iW(x_f, T^{(0)}; x_i, 0)/\hbar} \tag{131}$$

with

$$F(x_f, T^{(n)}; x_i, 0) = \left[2\pi\hbar\, p_(x_i) p_(x_f)\int_{x_i}^{x_f} \frac{dx}{p^3(x)}\right]^{-1/2} \tag{132}$$

as follows from the explicit form of $K(x_f, T; x_i, 0)$ in Eq. (124), $W(x_f, T^{(0)}; x_i, 0)$ - the phase factor (130) and $\gamma$ - the second derivative of the exponential in (122)

$$\gamma = \frac{\partial^2}{\partial T^2}\left(S[x_{cl}(t)] + ET\right) = -\frac{\partial E_{cl}(T)}{\partial T} \tag{133}$$

taken at $T^{(0)}$. Its explicit form is found by differentiating Eq. (102)

$$\begin{aligned} 1 &= \frac{\partial}{\partial T}\int_{x_i}^{x_f} dx\sqrt{\frac{m}{2(E_{cl}(T) - V(x))}} \;\rightarrow \\ &\rightarrow \quad \gamma = \left[\frac{m}{2}\int_{x_i}^{x_f} \frac{dx}{p^3(x)}\right]^{-1} \end{aligned}$$

Inserting the expressions for $F$ and $\gamma$ in Eq. (131) one obtains Eq. (129)

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Including all the saddle points $T^{(n)}$, Eq. (128) one obtains, Ref. [16],

$$G(x_f, x_i; E) = \sum_n G^{(n)}(x_f, x_i; E) \tag{134}$$

$$G^{(n)}(x_f, x_i; E) = \frac{m\hbar}{2\pi} \frac{(i\lambda)^n}{\sqrt{p_(x_i) p_(x_f)}} \exp \frac{1}{\hbar} \left[ \left( i \int_{x_i}^{a} + i \int_{b}^{x_f} - (2n+1) \int_{a}^{b} \right) p(x) dx \right].$$

with $\lambda$ - the turning point factor discussed in Refs. [16],[17] where it is shown that $\lambda = 1/2$.

### 3.2.2 Double well - instantons

### 3.2.3 Decay of a false ground state - bounce

# 4 Path Integrals in Statistical Mechanics

## 4.1 The density matrix and partition function

In this section we will extend the path integral formulation of statistical mechanics. Again for simplicity let us consider a one-dimensional problem with the Hamiltonian Eq. (29). Let us assume that the system is in a thermal equilibrium with a heat bath at temperature T. The fundamentals of statistical mechanics imply that such a system is described by the density operator[4]

$$\rho_{op}(\beta) = \frac{1}{Z(\beta)} e^{-\beta H_{op}} \tag{135}$$

where $\beta$ is the inverse temperature $\beta = 1/T$ and

$$Z(\beta) = Tr e^{-\beta H_{op}} = \sum_n e^{-\beta E_n} \tag{136}$$

is the partition function.[5]

[4]The details of the density operator formalism are discussed in a separate Chapter of this course. To follow the basics of the material presented here it should be sufficient to be familiar with the partition function

[5]In our notation $T$ is measured in energy units so there is no need for the Boltzmann constant $k_B$

Consider the coordinate matrix elements of $\rho_{op}(\beta)$

$$\langle x'|\rho_{op}(\beta)|x\rangle = \frac{1}{Z(\beta)}\langle x'|e^{-\beta H_{op}}|x\rangle \tag{137}$$

Comparing to the propagator $K(x', \Delta t; x, 0) = \langle x'|e^{-iH_{op}\Delta t/\hbar}|x\rangle$ one observes that apart of the $1/Z(\beta)$ normalization the two are formally related if one replaces $\Delta t$ in the propagator $K$ with imaginary time (often called Euclidean time) $\Delta t \to -i\hbar\beta$. With the path integral representation for $K$, this observation means that one can straightforwardly develop the path integral representing the matrix elements. $\langle x'|e^{-\beta H_{op}}|x\rangle$.

The procedure closely follows what we did for the propagator so we describe it briefly. Introducing

$$\eta = \frac{\beta\hbar}{N} \tag{138}$$

and representing

$$\langle x'|e^{-\beta H_{op}}|x\rangle = \langle x'|\underbrace{e^{-H_{op}\eta/\hbar}.....e^{-H_{op}\eta/\hbar}}_{N\,times}|x\rangle = \tag{139}$$

$$= \int dx_1 dx_2 ... dx_{N-1}\langle x'|e^{-H_{op}\eta/\hbar}|x_{N-1}\rangle\langle x_{N-1}|e^{-H_{op}\eta/\hbar}|x_{N-2}\rangle\ldots\langle x_1|e^{-H_{op}\eta/\hbar}|x\rangle$$

we can consider the limit of large $N \to \infty$ and use the expression (32) replacing infinitesimal $\epsilon$ by imaginary $-i\eta$

$$\lim_{\eta\to 0}\langle x_n|e^{-H_{op}\eta/\hbar}|x_{n-1}\rangle \approx \sqrt{\frac{m}{2\pi\hbar\eta}}\exp\left\{-\frac{1}{\hbar}\left[\frac{m(x_n - x_{n-1})^2}{2\eta} + \eta V(x_{n-1})\right]\right\} \tag{140}$$

to obtain

$$\begin{aligned}\langle x'|e^{-\beta H_{op}}|x\rangle &= \lim_{\eta\to 0}\left(\frac{m}{2\pi\hbar\eta}\right)^{N/2}\int\prod_{n=1}^{N-1}dx_n \\ &\times\exp\left\{-\frac{\eta}{\hbar}\sum_{n=0}^{N-1}\left[\frac{m(x_{n+1}-x_n)^2}{2\eta^2} + V(x_n)\right]\right\}\end{aligned} \tag{141}$$

and fixed $x_0 = x$, $x_N = x'$.

The exponent in the integrand of Eq. (141) is a discretized sum that in the limit $N \to \infty$ becomes the integral

$$S_E[x(\tau)] = \int_0^{\beta\hbar} d\tau\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)\right] \tag{142}$$

which is called Euclidian action with inverted sign of the potential $V(x)$ and $\tau$ denoting the imaginary time. In symbolic path integral notation

$$\begin{aligned}\langle x'|e^{-\beta H_{op}}|x\rangle &= \int_{x(0)=x}^{x(\beta\hbar)=x'} Dx[\tau]e^{-S_E[x(\tau)]/\hbar} = \\ &= \int_{x(0)=x}^{x(\beta\hbar)=x'} Dx[\tau]\exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)\right]\right\}\end{aligned} \tag{143}$$

The path integral for the partition function follows

$$Z(\beta) = Tre^{-\beta H_{op}} = \int dx_0\langle x_0|e^{-\beta H_{op}}|x_0\rangle = \int dx_0 \int_{x(0)=x_0}^{x(\beta\hbar)=x_0} Dx[\tau]e^{-S_E[x(\tau)]/\hbar} \tag{144}$$

where now as indicated the paths integrated over are those that start and end at the same coordinate point $x_0$ which is integrated over all possible values. So the integration is over a space of all possible closed paths.

## 4.2 High temperature limit

It is useful to consider the limit of high temperature $T$, i.e. small $\beta$. Then only closed paths $x(\tau)$ which do not deviate far from the initial point $x_0$ contribute. This is because in the short propagation "time" $\beta\hbar$ the path which deviate strongly must have a large velocity at the intermediate values of $\tau$. For such paths the integral of the kinetic energy in the Euclidian action $S_E$ will be large which will suppress the integrand exponentially. Therefore as a first approximation one can set $V(x) = V(x_0)$ in the integral in the exponent. Then the part of the exponent in Eq. (144) which contains the integral of the potential energy becomes

$$\exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau V(x)\right\} \approx \exp[-\beta V(x_0)] \tag{145}$$

and can be taken out of the path integral in Eq. (144) leaving the part which corresponds to a free particle

$$\begin{aligned}Z(\beta) &\approx \int dx_0 \exp[-\beta V(x_0)] \\ &\quad \times \int_{x(0)=x_0}^{x(\beta\hbar)=x_0} Dx[\tau]\exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\,\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2\right]\end{aligned} \tag{146}$$

This remaining path integral is easily found using the explicit expression (25) for the free particle propagator and substituting $x = x'$, $t - t' = -i\beta\hbar$. This gives

$$Z(\beta) \approx \frac{1}{\hbar}\sqrt{\frac{m}{2\pi\beta}}\int dx \exp[-\beta V(x)] = \int \frac{dxdp}{2\pi\hbar}\exp\left[-\beta\left(\frac{p^2}{2m} + V(x)\right)\right] \tag{147}$$

which is the expression for the classical partition function of the probabilities controlled by the Boltzmann factor $\sim \exp(-\beta H(p,x))$ to find the system in the phase space volume $dpdq$. This is measured in units $2\pi\hbar$ - the only remaining quantum mechanical element in this limit. of the exact expression.

DISCUSS THE COMPARISON OF THE CLASSICAL PHASE SPACE INTEGRAL AND THE PATH INTEGRAL IN THE EXACT EXPRESSION (144). THIS REFLECTS THE DIFFERENCE BETWEEN THE QUANTUM MECHANICAL AND CLASSICAL THERMAL FLUCTUATIONS.

MENTION THAT ONE CAN DERIVE A SYSTEMATIC EXPANSION OF QUANTUM CORRECTIONS TO THE CLASSICAL HIGH TEMPERATURE EXPRESSION - Wigner-Kirkwood expansion.

MENTION HOW TO DERIVE THE HIGH TEMPERATURE LIMIT OF THE THERMAL DENSITY MATRIX - NEED WIGNER TRANSFORM.

## 4.3 Example - thermal density matrix for harmonic oscillator

The known expression for the propagator of the harmonic oscillator, cf. Eqs. (64,67,77) when transformed to Euclidian time, $t_f - t_i = -i\beta\hbar$ gives the following expression for the corresponding thermal density matrix

$$\langle x'|\rho_{op}^{h.o.}(\beta)|x\rangle = \frac{1}{Z_{h.o}(\beta)}\langle x'|e^{-\beta H_{op}^{h.o}}|x\rangle = \tag{148}$$

$$= \frac{1}{Z_{h.o}(\beta)}\sqrt{\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}}\exp\left\{-\frac{m\omega}{2\hbar\sinh(\beta\hbar\omega)}\left[(x^2 + (x')^2)\cosh(\beta\hbar\omega) - 2x'x\right]\right\}$$

with the partition function

$$Z_{h.o}(\beta) = \int dx\langle x|e^{-\beta H_{op}^{h.o}}|x\rangle = \frac{1}{2\sinh(\beta\hbar\omega/2)} \tag{149}$$

Writing

$$Z_{h.o}(\beta) = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} = \sum_{n=0}^{\infty}\exp\left[-\beta\hbar\omega(n + 1/2)\right] \tag{150}$$

we obtain as expected the sum over all energy levels of the harmonic oscillator.

# 5 Appendix

## 5.1 Gaussian integrals

The basic integral is

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

from which

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \qquad \text{and} \qquad \int_{-\infty}^{\infty} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{b^2/4a}$$

follow by rescaling and completing the square.

## 5.2 Stationary phase approximation

### 5.2.1 One dimensional integrals

Let us start by considering a one dimensional integrals

$$\int_{-\infty}^{\infty} e^{isf(y)} dy \tag{151}$$

with the phase of the exponential in the integrand containing a large constant $s >> 1$. This means that it takes only a small change $\Delta y$ of $y$ to cause the phase change $s\Delta f \sim 2\pi$. The integrand therefore oscillates rapidly causing near cancellation as these oscillations are integrated over so the result is small. The exception are the points at which the phase is stationary, i.e. the roots of

$$\frac{df(y)}{dy} = 0 \tag{152}$$

In the vicinity of such stationary phase points the integrand changes slowly and one obtains a good approximation expanding the phase around these points. Assuming $y_c$ one of such points have

$$f(x) = f(y_c) + \frac{1}{2} f''(y_c)(y - y_c)^2 + ... \tag{153}$$

and the corresponding contribution to the integral

$$\int_{-\infty}^{\infty} e^{isf(y)} dy \approx e^{isf(y_c)} \int_{-\infty}^{\infty} e^{isz^2 f''(y_c)/2}\, dz = \sqrt{\frac{2\pi i}{sf''(y_c)}} e^{isf(y_c)} \tag{154}$$

where we used the Gaussian integrals expressions from Appendix 5.1. The above result assumes that the second derivative at the stationary point is not too small. Otherwise one must consider cubic order in the expansion. WE PLAN TO ADDRESS THIS BELOW IN THE CONTEX OF UNIFORM APPROXIMATION SECTION.

One must sum the above expression over all stationary points

$$\int_{-\infty}^{\infty} e^{isf(y)} dy \approx \sum_c \sqrt{\frac{2\pi i}{sf''(y_c)}} e^{isf(y_c)} \tag{155}$$

provided they are separated enough from each other. MENTION WHAT HAPPENS WHEN SOME OF THE STATIONARY POINTS ARE CLOSE - UNIFORM APPROXIMATION.

### 5.2.2 Generalizing to many variables

Let us now generalize the above to multidimensional integrals

$$\int d^M y e^{isf(y)} \text{ with } f(y) \equiv f(y_1, y_2, ..., y_M) \tag{156}$$

again assuming $s \gg 1$. In a similar manner as in one dimensional case the fast oscillations of the phase mean that the dominant contribution comes from the small vicinity of the stationary points which are now solutions of the M equations

$$\frac{\partial f(y)}{\partial y_k} = 0 \ , \ \ k = 1, ..., M \tag{157}$$

For each stationary point $y_c$ we expand to quadratic order in deviations $z = y - y_c$

$$f(y) \approx f(y_c) + \frac{1}{2} \sum_{jk} A_{jk} z_j z_k \text{ with } A_{jk} = \frac{\partial^2 f(y_c)}{\partial y_j \partial y_k} \tag{158}$$

With this approximation the contribution of the stationary phase point is given by the Gaussian integral

$$e^{isf(y_c)} \int d^M z \exp\left( \frac{is}{2} \sum_{jk} A_{jk} z_j z_k \right) \tag{159}$$

The matrix of second derivatives $A_{jk}$ is real symmetric and can be diagonalized using orthogonal transformation of the vector of the integration variables. Using the Dirac

notations we want to transform

$$z = O\xi \quad \rightarrow \quad \sum_{jk} A_{jk} z_j z_k \equiv \langle z|A|z\rangle = \langle \xi|O^T A O|\xi\rangle = \sum_{n=1}^{M} \lambda_n \xi_n^2 \tag{160}$$

with $\lambda_n$ the eigenvalues of $A$. The matrix $O$ which achieves this is built of the corresponding normalized and orthogonal eigenvectors. of the matrix $A$

$$Aa^{(n)} = \lambda_n a^{(n)} \quad \rightarrow \quad O_{nm} = a_m^{(n)} \quad \rightarrow \quad O^T O = I \tag{161}$$

Since $\det O = 1$ the change of variables $z \to \xi$ has $d^M z = d^M \xi$ and it transforms the stationary phase contribution into a product of 1-dimensional Gaussian integrals, cf., Eq. (154)

$$\begin{aligned} e^{isf(y_c)} \int d^M \xi \exp\left(\frac{is}{2} \sum_m \lambda_n \xi_n^2\right) &= \left(\frac{2\pi i}{s}\right)^{M/2} \left[\prod_{m=1}^{M} \lambda_m\right]^{-1/2} e^{isf(y_c)} = \\ &= \left(\frac{2\pi i}{s}\right)^{M/2} \left[\det \frac{\partial^2 f(y_c)}{\partial y_j \partial y_k}\right]^{-1/2} e^{isf(y_c)} \end{aligned} \tag{162}$$

Finally one must sum over all the stationary points

$$\int d^M y e^{isf(y)} \approx \left(\frac{2\pi i}{s}\right)^{M/2} \sum_c \left[\det \frac{\partial^2 f(y_c)}{\partial y_j \partial y_k}\right]^{-1/2} e^{isf(y_c)} \tag{163}$$

### 5.2.3 Saddle point generalization of the stationary phase method

## 5.3 Jacobian of the transformation Eq. (70)

Let us note that set the $\{u_n(t)\}$ in addition to orthonormality, Eq. (73) is complete in the space of functions $y(t)$

$$\sum_n u_n(t) u_n(t') = \delta(t - t') \tag{164}$$

We next note that the transformation (70) is linear so the Jacobian $\det \partial y_m / \partial a_n$ is a constant independent of $a_n$'s integration variables. To be more precise let us write the relations (164) and (73) in a discretized form with the usual notations as in e.g., Eq. (34),

$$\sum_n u_n(t_m) u_n(t_{m'}) = \frac{\delta_{mm'}}{\epsilon} \quad , \quad \epsilon \sum_m u_n(t_m) u_{n'}(t_m) = \delta_{nn'} \tag{165}$$

One observes that the matrix $O_{mn} \equiv \sqrt{\epsilon} u_n(t_m)$ (note the order of the indices) is orthogonal[6] according to the above relations, i.e.

$$OO^T = I \ , \ O^T O = I \tag{166}$$

Its determinant is therefore $\det O = 1$ which means that the Jacobian of the transformation Eq. (70) is

$$\det u_n(t_m) = \epsilon^{-(N-1)/2} \tag{167}$$

i.e. depends only on $\epsilon$.

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