PHY 305: WKB and Path Integral Formulation of QM

In these notes, we will study the relationship between quantum mechanics and classical mechanics. Any new physical theory that replaces an existing one, has to show that it can reproduce all the old results in the limit where the old theory is accurate. In our case, this limit is

\[ \hbar \to 0. \]

Since \( \hbar \) is a dimensionful quantity

\[ [\hbar] = \text{kg} \cdot \text{m}^2 \cdot \text{s}^{-1}. \]  \hspace{1cm} (1)

which is the units of angular momentum = momentum \( \times \) distance, or action = energy \( \times \) time. This means that the classical description should for systems for which the characteristic mass, size, and velocity are such that its ‘action’ is large compared to \( \hbar \). This important requirement is known as the correspondence principle, and quantum mechanics satisfies it beautifully.

1. Classical Action

For simplicity we consider a non-relativistic particle of mass \( m \) moving in one dimension, under influence of a potential \( V(x) \). We can describe the classical motion of the particle either via a Hamiltonian or a Lagrangian

\[ \begin{align*}
H(x, p) &= \frac{p^2}{2m} + V(x); \\
L(x, \dot{x}) &= \frac{1}{2}m\dot{x}^2 - V(x).
\end{align*} \]  \hspace{1cm} (2)

The equations of motion are respectively the Hamilton equations or the Euler-Lagrange equations

\[ \begin{align*}
\dot{x} &= \frac{\partial H}{\partial p}, \\
\dot{p} &= -\frac{\partial H}{\partial x}; \\
\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} &= 0.
\end{align*} \]  \hspace{1cm} (3)

In our specific example, these equations reduce to the familiar form

\[ \begin{align*}
\dot{x} &= \frac{p}{m}, \\
\dot{p} &= -\frac{\partial V}{\partial x}
\end{align*} \]  \hspace{1cm} (4)

which is just Newton’s equation with a force \( F(x) = -\frac{\partial V}{\partial x} \).
The usual formulation of quantum mechanics, via the Schrödinger equation and Heisenberg equations of motion, is most closely related to the Hamilton formulation of classical mechanics. In these notes, we will summarize an alternative formulation of quantum mechanics, the Feynman path integral formulation, that is more directly related to the Lagrangian formalism. The Hamiltonian and Lagrangian are related via a Legendre transformation:

\[ H(x,p) = p \dot{x} - L(x, \dot{x}) , \quad p = \frac{\partial L}{\partial \dot{x}} , \]  

\[ L(x, \dot{x}) = p \dot{x} - H(x,p) , \quad \dot{x} = \frac{\partial H}{\partial p} . \]  

(5) \hspace{1cm} (6)

On the right-hand side, one is instructed to eliminate the velocity \( \dot{x} \) in favor of the momentum \( p \) in the first equation, and eliminate \( p \) in favor \( \dot{x} \) in the second equation.

The Euler-Lagrange equation can be derived via the principle of least action. Consider a path \( x(t) \) that starts at position \( x_0 \) at time \( t_0 \) and ends at position \( x \) at time \( t \):

The action functional \( S \) is defined as the integral over time of the Lagrangian \( L(x, \dot{x}) \), evaluated over the whole path

\[ S = \int dt \, L(x, \dot{x}) \]  

(7)

Now consider a small deviation \( x(t) \rightarrow x(t) + \delta x(t) \) of this path. The variation of the action functional can be written as

\[ \delta S = \int dt' \left( \delta x(t') \frac{\partial L}{\partial x} + \delta \dot{x}(t') \frac{\partial L}{\partial \dot{x}} \right) \]

\[ = \int dt' \delta x(t') \left( \frac{\partial L}{\partial x} - \frac{d}{dt'} \frac{\partial L}{\partial \dot{x}} \right) + \int dt' \frac{d}{dt'} \left( \delta x(t') \frac{\partial L}{\partial \dot{x}} \right) \]

The first term on the right-hand side is zero for a classical path, that solves the Euler-Lagrange equations. The second term is a total time-derivative. So \( \delta S = 0 \), provided that the variation \( \delta x(t) \) vanishes at the end-points of the path. In case the variation \( \delta x(t) \) does not vanish at the end-points, we have

\[ \delta S = \delta x(t') \frac{\partial L}{\partial \dot{x}} \bigg|_{t_0}^t = \delta x(t) p(t) - \delta x_0 p(t_0) \]  

(8)
2. WKB Wavefunction

The equations of classical mechanics, as summarized above, are reproduced from the equations of quantum mechanics, by taking the classical limit $\hbar \to 0$. This is done as follows. As explained in Chapter 8 of Griffiths, the Schrödinger equation in the limit of small $\hbar$ is solved via the WKB approximation. To write the WKB wavefunction, we note that for a classical trajectory with energy $E$, the momentum $p$ can be solved as a function of position $x$ via

$$H(x,p) = E \rightarrow p = p(x), \quad p(x) \equiv \sqrt{2m(E - V(x))}. \quad (9)$$

The WKB wavefunction reads

$$\Psi_{WKB}(x,t) = \frac{C}{\sqrt{|p(x)|}} \exp \left( \frac{i}{\hbar} \left( \int_x^{x_0} p(x') dx' - E(t - t_0) \right) \right) \quad (10)$$

where $x_0$ is the position of the particle at some arbitrary initial time $t_0$.¹ In Griffiths it is shown that the above wavefunction solves the time-independent Schrödinger equation $H \Psi = E \Psi$. We now explain how it relates to classical mechanics.

Evaluating the action functional (7) for the classical trajectory $x(t)$ of energy $E$, going from $x_0$ at $t_0$ to position $x$ at time $t$, yields

$$S(x,t) = \int_{(x_0,t_0) \rightarrow (x,t)} (p \frac{dx}{dt} - H) dt = \int_{x_0}^x p(x') dx' - E(t - t_0) \quad (11)$$

where we used eqn (6). So we can write the WKB wavefunction as

$$\Psi_{WKB}(x,t) = \frac{C}{\sqrt{|p(x)|}} \exp \left( \frac{i}{\hbar} S(x,t) \right) \quad (12)$$

So we conclude that:

the phase factor of the WKB wavefunction $\Psi_{WKB}(x,t)$ is $1/\hbar$ times the action functional $S$ evaluated along the classical path that ends at position $x$ at time $t$.

Note that via the WKB wavefunction (12), we can relate the quantum mechanical definition $p = \hbar \frac{\partial}{\partial x}$ to the classical identity $p(x) = \frac{\partial S}{\partial x}$, which can be derived from eqns (8) or (11).

¹Different choices for $t_0$ just change the wavefunction by an overall constant independent of $x$ and $t$. 
3. Feynman Path Integral

The Feynman path integral is a reformulation of quantum mechanics, that makes use of
the Lagrangian formulation of classical mechanics. One of its advantages is that it can be
applied more easily to relativistic theories, and to quantum field theories. Here we summarize
how it works for a non-relativistic particle in one dimension. Consider the following question:

At time $t_0$ the particle is located at $x_0$, what is the probability that at time $t$ it is located at $x$?

In the usual formulation of quantum mechanics, we would answer this question as follows.
At time $t_0$ the particle, the particle is in the position eigenstate $|x_0\rangle$. The wavefunction
$\Psi(x,t)$ that solves the Schrödinger equation, with this initial condition, is

$$\Psi(x,t) = \langle x | e^{-\frac{i}{\hbar}(t-t_0)H} | x_0 \rangle$$

(13)

The probability to be at the location $x$ at time $t$ is equal to the absolute value squared of this
wavefunction. Or more accurately, the probability to be between $x$ and $x+dx$ is $|\Psi(x,t)|^2 dx$.

As a short warm-up exercise, let us compute $\Psi(x,t)$ in the case of a free particle with
Hamiltonian $H = p^2/2m$. Since the Hamiltonian is just a function of the momentum, it is
most convenient to solve the Schrödinger equation in the momentum representation. To do
this, we insert into eqn (13) twice the closure relation

$$1 = \int dp |p\rangle\langle p|$$

(14)

where $1$ is the identity operator. So we write

$$\Psi(x,t) = \int dp \int dp_0 \langle x | p \rangle \langle p | e^{-\frac{i}{\hbar}(t-t_0) \frac{p^2}{2m}} | p_0 \rangle \langle p_0 | x_0 \rangle$$

Using

$$\langle p | p_0 \rangle = \delta(p-p_0), \quad \langle p | x \rangle = \frac{e^{i\frac{p}{\hbar}x}}{\sqrt{2\pi\hbar}}$$

(15)

we can easily perform the momentum integral and find

$$\Psi(x,t) = \sqrt{\frac{im}{2\pi\hbar(t-t_0)}} \exp\left(\frac{i}{\hbar} \frac{m(x-x_0)^2}{2(t-t_0)}\right)$$

(16)

The phase in the exponent equals $1/\hbar$ times the action $S(x,t)$ of the path from $x_0$ to $x$. 

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Now let us turn to the derivation of the Feynman path integral formula. Schematically, it reads as follows

$$\langle x | e^{-\frac{i}{\hbar}(t-t_0)H} | x_0 \rangle = \sum_{\text{paths } x(t')} e^{i\frac{\hbar}{\hbar}S(x(t'))}$$ (17)

The sum on the right-hand side is over all trajectories $x(t')$ that start at $x_0$ at time $t_0$ and end at $x$ at time $t$, and $S(x(t'))$ is the action functional (7) evaluated for the trajectory $x(t')$.

To derive this formula, we start by dividing the time interval between the initial time $t_0$ and final time $t$ into $N$ small time intervals of size $\Delta t$ such that

$$t - t_0 = N\Delta t$$ (18)

Correspondingly, we can write

$$e^{-\frac{i}{\hbar}(t-t_0)H} = e^{-\frac{i}{\hbar}N\Delta t H} = \underbrace{e^{-\frac{i}{\hbar} \Delta t H} e^{-\frac{i}{\hbar} \Delta t H} \cdots e^{-\frac{i}{\hbar} \Delta t H}}_{N \text{ times}}$$ (19)

Define $t_n = t_0 + n\Delta t$, and denote the position $x(t_n)$ at this instant by $x_n$. So $(x_N, t_N) = (x, t)$.

As indicated by eqn (18) and the above figure, the idea is to divide the time evolution from $t_0$ to $t$ into $N$ small time intervals, and first do the compute the amplitude for each separate small step

$$\langle x_{n+1} | e^{-\frac{i}{\hbar} \Delta t H} | x_n \rangle$$ (20)

Then afterwards, we will glue all small steps together by repeated use of the formula

$$\langle x_{n+1} | e^{-\frac{i}{\hbar} 2\Delta t H} | x_{n-1} \rangle = \int dx_n \langle x_{n+1} | e^{-\frac{i}{\hbar} \Delta t H} | x_n \rangle \langle x_n | e^{-\frac{i}{\hbar} \Delta t H} | x_{n-1} \rangle$$ (21)

This gluing identity uses the closure formula $1 = \int dx |x \rangle \langle x |$. Eventually, we will take the limit $N \to \infty$, $\Delta t \to 0$, while keeping the product (18) fixed.
Let us evaluate the matrix element \(20\).

\[
\langle x_{n+1} | e^{-\frac{i}{\hbar} \Delta t H} | x_n \rangle = \int dp_n \langle x_{n+1} | p_n \rangle \langle p_n | e^{-\frac{i}{\hbar} \Delta t H(x, p)} | x_n \rangle
\]

\[
= \int dp_n \frac{e^{\frac{i}{\hbar} p_n x_{n+1}}}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar} (p_n x_n + H(x, p_n) \Delta t)} \frac{1}{\sqrt{2\pi\hbar}}
\]

\[
= \int dp_n \frac{\delta}{\sqrt{2\pi\hbar}} \int \frac{dx}{\sqrt{2\pi\hbar}} e^{i\frac{\Delta t}{\hbar} \left( p_n \frac{x_{n+1} - x_n}{\Delta x} - H(x, p_n) \right)}
\]

In the first step we used eqn (14), the second eqn (15) and that \(\langle p_n | H(x, p) | x_n \rangle = H(x, p_n)\). Performing the Gaussian integral over \(p_n\) is easy (see eqn (16)), but we prefer to save this momentum integral for later.

We can now put it all together. First we multiply the exponentials we just found in eqn (22) over all the \(N\) small steps. In the large \(N\) limit, we can rewrite this product as

\[
\lim_{N \to \infty} \prod_{n} e^{\frac{i}{\hbar} \Delta t \left( p_n \frac{x_{n+1} - x_n}{\Delta x} - H(x, p_n) \right)} = \exp \left( \frac{i}{\hbar} \int_{t_0}^{t} dt' \left( p \dot{x} - H(x, p) \right) \right)
\]

In the exponential, we recognize the expression eqn (6) for the Lagrangian \(L = p \dot{x} - H(x, p)\). Next, in gluing together all the steps, we have to integrate over all the intermediate positions \(x_n\). We also still have to do the integrals over all the intermediate momenta \(p_n\) in (22). Multiplying all these integrals together gives

\[
\lim_{N \to \infty} \prod_{n} \int dx_n dp_n = \int \mathcal{D}x \mathcal{D}p
\]

The left-hand side represents an addmittedly somewhat formal limit, but we will work with it anyway. The symbol on the right-hand side is interpreted as the integral over all particle trajectories \((x(t'), p(t'))\) that connect the initial situation \((x_0, t_0)\) to the final situation \((x, t)\).

The final result is the Feynman path integral formula

\[
\langle x | e^{-\frac{i}{\hbar} (t-t_0) H} | x_0 \rangle = \int \mathcal{D}x \mathcal{D}p e^{\frac{i}{\hbar} \int_{t_0}^{t} dt' \left( p \dot{x} - H(x, p) \right)}
\]

Performing the Gaussian integral over \(p(t)\), using eqn (6), gives (dropping an overall constant)

\[
\langle x | e^{-\frac{i}{\hbar} (t-t_0) H} | x_0 \rangle = \int \mathcal{D}x e^{\frac{i}{\hbar} \int_{t_0}^{t} dt' L(x, \dot{x})}
\]
4. Semi-classical limit

It is instructive to compare the Feynman path integral formula (26) with the expression (12) for the WKB wave function. Both formulas express $\Psi(x, t)$ in terms of the exponential of $1/\hbar$ times the action $S(x, t)$ of the path from the initial position $x_0$ at time $t_0$ to the final position $x$ at time $t$. In the path integral formula, however, sums over all possible paths, whereas the WKB formula only involves one single classical path. Correspondingly, the path integral formula is an exact description of the wave function, whereas the WKB formula is accurate only in the so-called semi-classical limit, i.e. when $\hbar$ is very small.

An intuitive way to understand how the WKB answer arises from the path integral formula is as follows. When $\hbar$ is very small, the exponential $e^{iS/\hbar}$ is a rapidly oscillating functional on the space of possible paths. Because of these rapid oscillations, most contributions will cancel each other out in the sum over all possible paths. Only near the special paths where the action $S$ is stationary, that is, for the paths that minimize the action $S$, the phase factor $e^{iS/\hbar}$ varies sufficiently slowly, so that constructive interference can occur. The paths for which $S$ is stationary are of course just the classical paths, that solve the Euler-Lagrange equation of motion. For small $\hbar$ we can therefore accurately approximate the integral over all paths by keeping only the contributions of paths very close to the classical path, for which the action is stationary. This approximation is called the stationary phase approximation, or semi-classical approximation.

5. Double Well Potential

As an application of the WKB approximation, we now discuss the double well potential

$$V(x) = \frac{1}{8} \lambda (x - a)^2 (x + a)^2$$  (27)

This potential has two minima, at $x = -a$ and at $x = a$, separated by a potential barrier as indicated in the figure below:
Near the two minima \( x = \pm a \), the potential \( V(x) \) is well approximated by a harmonic oscillator potential. We are interested in answering the following question:

At \( t = 0 \), the particle is in the lowest energy state inside the left well, what is the probability that at a later time \( t \) the particle has tunneled through the barrier and sits in the right well?

The answer to this question is found by considering the lowest two energy states of the system. They are given by an even and odd wavefunction \( \Psi^\pm(x) \), that both reduce (to a very good approximation) to the harmonic oscillator ground states in each well. Here \( \Psi^+ \) is even and \( \Psi^- \) is odd under the reflection \( x \rightarrow -x \). The corresponding energy levels \( E^\pm \) are split by a small amount

\[
E^\pm = E_0 \mp \hbar \epsilon , \quad E_0 = \frac{1}{2} \hbar \omega , \quad \omega = \sqrt{\frac{\lambda a^2}{m}} .
\]

(28)

Using the even and odd energy eigenstates \( \Psi^\pm \), we can construct a left and right ground state via

\[
\Psi_{\text{left}} = \frac{1}{\sqrt{2}}(\Psi^+ + \Psi^-) , \quad \Psi_{\text{right}} = \frac{1}{\sqrt{2}}(\Psi^+ - \Psi^-) .
\]

(29)

The left and right state both have an energy that is close to \( E_0 \), but neither is an exact energy eigenstate. So if at \( t = 0 \), the state is equal to \( \Psi_{\text{left}} \), it will evolve non-trivially in time into a state of the form (see eqn (28))

\[
\Psi(t) = e^{-\frac{i}{\hbar}E_0 t} \left( \Psi_{\text{left}} \cos(\epsilon t) + \Psi_{\text{right}} \sin(\epsilon t) \right) .
\]

(30)

So the probability to end up in the right well at time \( t \) is

\[
P(t) = |\sin(\epsilon t)|^2
\]

(31)

Now clearly, in case the potential barrier is high relative to the ground state energy \( E_0 \), we expect the probability \( P(t) \) to be very small, at least at early times.\(^2\) Concretely, we expect that \( \epsilon \) is roughly proportional to the amplitude for tunneling through the potential barrier. Using the WKB approximation, and the fact that \( E_0 \ll V_{\text{barrier}} \), we can estimate

\[
\epsilon \sim e^{-S_0/\hbar} , \quad S_0 = \int_{-a}^{a} dx \sqrt{2mV(x)} .
\]

(32)

Here \( S_0 \) can in fact be interpreted as the classical action of the tunneling trajectory, defined as indicated in the figure below:

\(^2\)Note that after a time of order \( \pi/\epsilon \), the probability of finding the particle in the right well is equal to 1!
What is the meaning of this tunneling trajectory? Clearly, it is not a true classical trajectory, since tunneling is not allowed classically. Instead, tunneling arises because the Schrödinger equation allows for solutions in which the WKB momentum \( p(x) \) takes an imaginary value. Imaginary momentum is like imaginary velocity, or equivalently, the velocity of a motion that takes place during an imaginary time interval. If we replace \( t \) by \( it \), it flips the sign of the kinetic energy \( T = \frac{1}{2} m \dot{x}^2 \). In the Euler-Lagrange equations, this has the same effect as flipping the sign of the potential \( V(x) \), while keeping the sign of \( T \) fixed. With \( V(x) \) turned upside down, the two minima at \( x = \pm a \) become two maxima. The left and right ground states describe the situation where the particle is balanced at the respective maximum. The tunneling trajectory, whose classical action is given by eqn (32), corresponds to the classical motion of the ball rolling from the left maximum to the right maximum.\(^3\)

The result (32) can be derived using the WKB approximation. In the intermediate region, where the particle is tunneling between the two potential wells, we can approximate the even and odd wavefunction \( \Psi^\pm \) via the WKB approximation as

\[
\psi_{\text{WKB}}^\pm(x) = \frac{C^\pm}{|p(x)|} \left( e^{\frac{i}{\hbar} \int_0^x |p(x')| \, dx'} \pm e^{-\frac{i}{\hbar} \int_0^x |p(x')| \, dx'} \right),
\]

\[p(x) = \sqrt{2m(V(x) - E_0)}\]  

Note that in the neighborhood of \( x = \pm a \), we can approximate the double well potential \( V(x) \) by a simple harmonic potential \( V_{\pm}(x) = \frac{1}{2} m \omega^2 (x \mp a)^2 \). The ground state wave functions in these two harmonic well are\(^4\)

\[
\psi_{\text{left}}(x) = e^{-\frac{m \omega^2}{2\hbar} (x + a)^2}, \quad \psi_{\text{right}}(x) = e^{-\frac{m \omega^2}{2\hbar} (x - a)^2}.
\]

\(^3\)In relativistically invariant theories, replacing \( t \) by \( it \) changes the 4-d Minkowski space into a 4-d Euclidean space. A tunneling trajectory is therefore often called a Euclidean trajectory.

\(^4\)Here we arbitrarily fix the normalization of the wave function such that \( \Psi^\pm(\pm a) = \pm 1 \). The probability density is thus obtained via \( P(x) = |\Psi(x)|^2 / \langle \Psi |^2 \rangle \), where the norm squared is defined by \( \langle \Psi \rangle^2 = \int dx |\Psi(x)|^2 \).
The idea is to evaluate $\Psi_{\text{WKB}}^\pm$ in the regions near the left and right harmonic wells, and to compare them with the above two ground state wave functions. Since the situation is symmetric, we only need to consider one of the two regions, say, the right well near $x = a$. Using that $E_0 = \frac{1}{2}\hbar \omega$ is small, we can approximate the WKB integral in this region as follows

$$\frac{1}{\hbar} \int_0^x dx' p(x') \simeq \frac{1}{2\hbar} S_0 - \frac{m\omega}{2\hbar}(x-a)^2 - \frac{1}{2} \log\left(\frac{a-x}{b}\right)$$  \hspace{1cm} (36)$$

Here $S_0$ is the action of the tunneling trajectory given in eqn (32), and $b$ is some constant, whose value will not be very important to us. Using this result, we find that the WKB wave function in the right harmonic well takes the following form$^5$

$$\psi_{\text{WKB}}^\pm(x) \simeq \pm e^{-\frac{m\omega}{2\hbar}(x-a)^2} + b e^{-\frac{1}{\hbar}S_0} e^{\frac{m\omega}{2\hbar}(x-a)^2}$$  \hspace{1cm} (37)$$

We see that the difference between the WKB wave function and the harmonic ground state wave function is proportional to the $e^{-S_0/\hbar}$. With some more work one can show that $\Psi_{\text{WKB}}^\pm(x)$ solves the time-independent Schrödinger equation with energy $E^\pm$ as given in eqn (28), where $\epsilon$ as estimated in eqn (33). We will not do the precise calculation here, since the leading order estimate (33) for $\epsilon$ is already evident from eqn (37).

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$^5$Here we fixed the constants $C_\pm$ such that the WKB wave function matches the normalization (33) of the left and right wave functions.