FYS 4110/9110 Modern Quantum Mechanics
Midterm Exam, Fall Semester 2024

Return of solutions:
The problem set is available from Friday morning, 27 September.
You may submit handwritten solutions, but they have to be scanned and included in one single file, which is submitted in Inspera before Friday, 4 October, at 14:00.

Language:
Solutions may be written in Norwegian or English depending on your preference

Questions concerning the problems:
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To aid you in solving the problems, you may consult any material that you can find on the topic, but as always you should cite the sources you use.

Problem 1: WKB approximation

In this problem we are going to derive the WKB approximation for solving the Schrödinger equation. We study a particle moving in one dimension, with the potential energy $V(x)$, giving the time-independent Schrödinger equation for the wavefunction $\psi(x)$,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi.$$

a) Starting from the Schrödinger equation, write the wavefunction in the form $\psi(x) = Ae^{i\phi}$ (with A and ϕ real functions of x) and derive the equations

$$A'' = A\left(\phi'^2 - \frac{p^2}{\hbar^2}\right)$$
$$2A'\phi' + A\phi'' = 0$$

Here the prime denotes derviative with respect to x and

$$p(x) = \sqrt{2m((E - V(x))}$$

is the classical momentum of a particle with energy E at the position x.

If the potential energy is constant, we know that the solution to the Schrödinger equation is a plane wave. The idea behind the WKB approximation is that if the potential energy changes slowly compared to the wavelength, the wave function will be almost a plane wave, but with slowly changing amplitude and wavelength. In the equations, this is implemented by assuming that if $\frac{A''}{A} \ll \phi'^2, \frac{p^2}{\hbar^2}$, we can neglect the term with A'' in the equations. This is called the WKB approximation.

b) Show that under this assumption, there will be two independent solutions

$$\psi_\pm = \frac{1}{\sqrt{p}} e^{\pm \frac{i}{\hbar} \int p dx} \tag{1}$$

with the general wavefunction being a linear combination of these.

c) The classical turning points are the points were $V(x) = E$, which means $p(x) = 0$. Explain why the WKB approximation will fail close to the classical turning points.

To simplify the equations, we assume for the moment that the turning point is at $x = 0$ when the energy is E. The WKB solution (1) then provides a good approximation to the true wavefunction when $x \ll 0$ and $x \gg 0$, but not when x is close to 0.

d) Assume that the potential is increasing close to $x = 0$, so that $V'(0) > 0$. Explain why the general solution far from 0 is of the form

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{p}} \left[B e^{\frac{i}{\hbar} \int_x^0 p(x')dx'} + C e^{-\frac{i}{\hbar} \int_x^0 p(x')dx'} \right] & x < 0 \\ \frac{1}{\sqrt{|p|}} D e^{-\frac{1}{\hbar} \int_0^x |p(x')|dx'} & x > 0 \end{cases} \tag{2}$$

To find an approximate wavefunction close to the turning points, we can approximate the potential as linear in the vicinity of the turning point. The potential energy is then approximately $V(x) = E + V'(0)x$.

e) Defining

$$\alpha = \sqrt[3]{\frac{2mV'(0)}{\hbar^2}}, \qquad z = \alpha x,$$

show that the Schrödinger equation is

$$\frac{d^2\psi_p}{dz^2} = z\psi_p. \tag{3}$$

Here $\psi_p(x)$ is an approximation to the true wavefunction that will be accurate close to the turning point $x = 0$.

Equation (3) is known as the Airy equation. Being a second order equation it has two independent solutions, which are called the Airy functions $Ai(z)$ and $Bi(z)$. The general solution close to the turning point is then the linear combination

$$\psi_p(x) = aAi(\alpha x) + bBi(\alpha x). \tag{4}$$

The idea is now to match the solution ψ_p to the solution $\psi(x)$ from Eq (2) in the region that is far enough from the turning point so that $\psi(x)$ is accurate, while still close enough to the turning point to allow the potential to be approximated as linear, so that $\psi_p x)$ is also accurate. You could worry that no such region exists, and there are cases where it does not. We will not go into this question, but assume that it is possible to find a region where both solutions are accurate. You will numerically confirm this below for the harmonic oscillator. To match the solutions, we need the asymptotic form of the Airy functions for large z.

f) Search for information on the Airy functions, and find the expressions for the asymptotic form for large z (you do not have to derive these expressions, just cite your sources).

g) Show that the the two solutions (2) and (4) match if

$$a = \sqrt{\frac{4\pi}{\hbar\alpha}}D, \qquad b = 0,$$
$$B = -ie^{i\pi/4}D, \qquad C = ie^{-i\pi/4}D.$$

h) Repeat the matching procedure for a turning point where $V' < 0$ and show that if we have a potential with a minimum we can have bound states with energy E provided

$$\int_{x_1}^{x_2} p(x')dx' = (n\pi - \frac{\pi}{2})\hbar, \qquad n = 1, 2, 3, \dots$$

i) Determine the energy levels in the WKB approximation for the harmonic oscillator with Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2.$$

j) For the harmonic oscillator, plot the WKB wave functions in the various regions for one or more of the energy eigenstates. Include also in the figure the exact eigenfunction for comparison. Part of the aim of this question is that you should select parameters so that you illustrate in a clear way the nature of the solution.

Problem 2: Semiclassical approximation to the path integral

The WKB approximation gives the exact energy levels for the harmonic oscillator. Looking at the wavefunctions, it is not clear why this happens, since the wavefunctions are not exact (even if they are quite accurate approximations). In this problem, we are going to derive the same semiclassical quantization condition from the path integral and in the process see that for a quadratic Lagrangian (as in the harmonic oscillator) we will not make any approximation, thus explaining why we get the exact energy eigenvalues.

We start from the path integral expression for the propagator

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

where

$$S[x(t)] = \int_{t_i}^{t_f} dt L(x, \dot{x}), \qquad L(x, \dot{x}) = \frac{1}{2}m\dot{x}^2 - V(x).$$

The classical solution $x_c(t)$ is the one where the action is stationary, $\delta S[x_c(t)] = 0$. Write $x(t) = x_c(t) + y(t)$, where the deviation from the classical solution is constrained by $y(t_i) = y(t_f) = 0$.

a) Show that

$$S[x(t)] = S[x_c] + \int_{t_i}^{t_f} dt \left[\frac{1}{2}m\dot{y}^2 - \frac{1}{2}V''(x_c)y^2\right] + \text{ Terms with } y^3 \text{ or higher.} \tag{5}$$

b) The semiclassical approximation consists in keeping only the terms up to order y^2. Show that the semiclassical approximation to the propagator is

$$G(x_f, t_f; x_i, t_i) = e^{\frac{i}{\hbar}S[x_c]} \int_{y(t_i)=0}^{y(t_f)=0} \mathcal{D}y(t) e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\left[\frac{1}{2}m\dot{y}^2 - \frac{1}{2}V''(x_c)y^2\right]}. \tag{6}$$

The path integral in Eq (6) is that of a Lagrangian

$$L = \frac{1}{2}m\dot{y}^2 - \frac{1}{2}V''(x_c)y^2$$

which we recognize as that of a harmonic oscillator. However, since x_c is a function of time, it is a harmonic oscillator with a time dependent frequency. Solving this problem involves some ad-hoc tricks, which we will not discuss. It can be shown that

$$\int_{y(t_i)=0}^{y(t_f)=0} \mathcal{D}y(t) e^{-\frac{i}{\hbar}\frac{m}{2}\int_{t_i}^{t_f} dt y\left[\frac{d^2}{dt^2} + W(t)\right]y} = \sqrt{\frac{m}{2\pi i\hbar f(t_i) f(t_f) \int_{t_i}^{t_f} \frac{dt}{f^2(t)}}} \tag{7}$$

where $f(t)$ is any solution of the equation

$$\left[\frac{d^2}{dt^2} + W(t)\right] f(t) = 0$$

with initial condition $f(t_i) \neq 0$. You are not to show this, but can use it in the following.

c) Check that Eq (7) gives the known propagators for the free particle and the harmonic oscillator for specific choices of $W(t)$ and $f(t)$.

We want to extract the spectrum of eigenvalues from the propagator. In the lectures, we derived the relation

$$G(x_f, t_f; x_i, t_i) = \sum_n \phi_n(x_f)\phi_n^*(x_i) e^{-\frac{i}{\hbar}E_n T}$$

where $T = t_f - t_i$ and E_n are the energy eigenvalues so that

$$H|n\rangle = E_n|n\rangle$$

with the energy eigenstates $|n\rangle$ in the position basis being $\phi_n(x) = \langle x|n\rangle$. We define the trace of the propagator

$$G(T) = \int dx_0 G(x_0, t_f; x_0, t_i) \tag{8}$$

and it's one sided Fourier transform

$$G(E) = \frac{i}{\hbar}\int_0^\infty dT e^{\frac{i}{\hbar}ET} G(T). \tag{9}$$

d) Show that

$$G(T) = \sum_n e^{-\frac{i}{\hbar}E_n T} \tag{10}$$

and

$$G(E) = \sum_n \frac{1}{E_n - E}. \tag{11}$$

e) Apply Eqs (8) and (10) to the harmonic oscillator (look up the propagator), and check that they give the correct energy levels.

f) We now want to apply Eq (7) to the path integral in Eq (6). Show that in this case we can choose $f(t) = \dot{x}_c(t)$, so that we then get

$$G(T) = \int dx_0 e^{\frac{i}{\hbar}S[x_c]} \sqrt{\frac{m}{2\pi i\hbar \dot{x}_c(0)\dot{x}_c(T)\int_0^T \frac{dt}{\dot{x}_c^2}}}. \tag{12}$$

In the integral over x_0 in (12), there will be some classical solutions where the action is independent of x_0 (so that $\frac{d}{dx_0}S[x_c] = 0$). These will give large contributions to the integral, while all the other classical solutions will give rapidly oscillating terms that will average to 0. We will therefore only retain the classical solutions that have action independent of x_0.

g) Show that these are the periodic solutions. You may use the following fact from classical mechanics: The action on the classical solution is a function of the initial and final position, as well as the time interval, $S[x_c] = S(x_f, T; x_i, 0)$. Then

$$\frac{\partial S}{\partial x_f} = p_f, \qquad \frac{\partial S}{\partial x_i} = -p_i$$

where p_i and p_f are the initial and final momenta.

For a given T, we will get contributions from all classical solutions with period T/n for some integer n. We call this classical solution $x_{T/n}(t)$, and get that

$$G(T) = \int dx_0 \sum_{n=1}^{\infty} e^{\frac{i}{\hbar}nS_{T/n}} \sqrt{\frac{m}{2\pi i\hbar}} \frac{1}{|\dot{x}_{T/n}(0)|} \left[\int_0^T \frac{dt}{\dot{x}_{T/n}^2}\right]^{-1/2} \tag{13}$$

where $S_{T/n}$ is the action evaluated for one period of time T/n.

h) Explain why both $S_{T/n}$ and $\int_0^T \frac{dt}{\dot{x}_{T/n}^2}$ are independent of x_0, so that the only x_0 dependency is in the term $\dot{x}_{T/n}(0)$. Show that

$$\int dx_0 \frac{1}{|\dot{x}_{T/n}(0)|} = \frac{T}{n}.$$

One can show that

$$\left[\int_0^T \frac{dt}{\dot{x}_{T/n}^2}\right]^{1/2} = (-1)^n \sqrt{-m\frac{dT}{dE_{T/n}}}$$

where $E_{T/n}$ is the energy of the solution $x_{T/n}(t)$. You do not have to show this, but use it in the following.

i) By changing the integration variable from T to $u = T/n$, show that

$$G(E) = \frac{i}{\hbar}\sqrt{\frac{i}{2\pi\hbar}}\sum_n (-1)^n \int_0^\infty du e^{\frac{i}{\hbar}n(Eu+S_u)} u\sqrt{n}\left(\frac{dE_u}{du}\right)^{1/2}.$$

The stationary phase approximation is used to extract the leading term in the asymptotic expansions of certain integrals. For large κ, we have that

$$\int_a^b f(x)e^{i\kappa g(x)}dx \approx \sqrt{\frac{2\pi}{\kappa}}\sum_{j=1}^{n}\frac{e^{\pm i\pi/4}}{\sqrt{|g''(x_j)|}}f(x_j)e^{i\kappa g(x_j)} \tag{14}$$

where the sum is over all the stationary points of the exponent ($g'(x_j) = 0$) that are inside the limits of integration and the sign is $\pm$ according as $g''(x_j) \gtrless 0$.

j) Use the stationary phase approximation with $1/\hbar$ as the large parameter and show that

$$G(E) = \frac{i}{\hbar}\sum_n (-1)^n e^{\frac{i}{\hbar}nW} u_0$$

where $u_0(E)$ found as the solution of $E - E_{u_0} = 0$ and $W = S_{u_0} + Eu_0$. You may use without proof that $\frac{dS_u}{du} = -E_u$ and $\frac{d^2S_u}{du^2} = -\frac{dE_u}{du}$.

k) Calculate the sum of the above series. According to Eq (11) the poles of $G(E)$ give the energy eigenvalues. Use this to derive the quantization condition

$$\int_{x_1}^{x_2} p(x')dx' = \pi\hbar(n+\frac{1}{2}), \qquad n = 0, 1, 2, \ldots.$$

Problem 3: Comparing the two approximations

We have derived the same quantization condition

$$\int_{x_1}^{x_2} p(x')dx' = (n\pi - \frac{\pi}{2})\hbar, \qquad n = 1, 2, 3, \ldots$$

both from the WKB approximation and the semiclassical approximation to the path integral. In this small final problem we will explore some arguments for why we arrive at the same result from two different staring points. The main observation is that both approximations can be understood as the lowest order of expansions in powers of $\hbar$, and that therefore it is not so surprising that they give the same result.

a) We can derive the WKB approximation in a different way than the one we used before. Write the wavefunction as

$$\psi(x) = e^{\frac{i}{\hbar}f(x)}$$

where $f(x)$ now is a complex function, so this form is completely general. Show that $f(x)$ satifies the equation

$$i\hbar f'' - f'^2 + p^2 = 0$$

b) Write $f(x) = f_0(x) + \hbar f_1(x) + \hbar^2 f_2(x) + \cdots$ as a power series in $\hbar$. Show that if we keep only terms up to first order in $\hbar$ we get the WKB wavefunctions

$$\psi_\pm = \frac{1}{\sqrt{p}} e^{\pm \frac{i}{\hbar} \int p dx}$$

c) To see that also the semiclassical approximation to the path integral can be considered the first term in an expansion in powers of $\hbar$, we go back to the expansion (5) of the action in powers of y, which we will now write in the form

$$S[x(t)] = S[x_c] + \Delta S_2(y^2) + \Delta S_3(y^3) + \cdots .$$

By changing variables in the path integral to $z(t) = y(t)/\sqrt{\hbar}$, show that in the limit where $\hbar \to 0$, the contribution of the ΔS_3 term and higher order terms become small compared to the second order term.