FYS4110 Midterm Exam

Aleksander Sekkelsten
Faculty of Mathematics and Natural Sciences, University of Oslo

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Task 1 — WKB approximation

In this problem I will perform the WKB approximation on the Schrödinger equation for a particle in a potential:

$$\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

Part a)

Problem Statement:

Starting from the Schrödinger equation, write the wavefunction in the form $\psi(x) = Ae^{i\phi(x)}$, where both A and ϕ are real functions of x. Derive the following equations:

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

Here the prime denotes derivatives with respect to x, and the classical momentum of a particle with energy E at position x is given by:

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

Solution:

Now, we make an ansatz $\psi = A(x)e^{i\phi(x)}$ and evaluate the Schrödinger equation. We get for the first term :

$$\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = \frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}A(x)e^{i\phi(x)} = \frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left[A'(x)e^{i\phi(x)} + iA(x)\phi'(x)e^{i\phi(x)}\right] =$$
$$\frac{\hbar^2}{2m}\left(A''(x)e^{i\phi(x)} + 2iA'(x)\phi'(x)e^{i\phi(x)} + iA(x)\phi''(x)e^{i\phi(x)} - A(x)\phi'^2(x)e^{i\phi(x)}\right)$$

For the full Schrödinger equation, we will get one Real part, and one imaginary part, which must satisfy the equation separately. Therefore we get the real term:

$$\frac{\hbar^2}{2m}\left(A''(x)e^{i\phi(x)} - A(x)\phi'^2(x)e^{i\phi(x)}\right) = (E - V(x))Ae^{i\phi(x)} \to A'' = A\left(\phi'^2 - \frac{p^2}{\hbar^2}\right)$$

and the imaginary term which reduces only to:

$$\frac{\hbar^2}{2m}2iA'(x)\phi'(x)e^{i\phi(x)} + iA(x)\phi''(x)e^{i\phi(x)} = 0 \to 2A'\phi' + A\phi'' = 0$$

Part b)

Problem Statement:

Under the assumption that $\frac{A''}{A} \ll \phi'^2 - \frac{p^2(x)}{\hbar^2}$*, show that there are two independent solutions:*

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

Solution:

Now We make an approximation, assuming that

$$\frac{A''}{A} \ll \phi' - \frac{p^2}{\hbar^2} \to \left(\frac{\partial}{\partial x}\phi(x)\right) \approx \frac{p^2}{\hbar^2} \to \int \frac{\partial}{\partial x}\phi(x) dx = \pm \int \frac{p}{\hbar} dx \to \phi(x) = \pm \frac{1}{\hbar} \int p dx$$

$$2A'\phi' + A\phi'' = 0 \to 2A'\frac{p}{\hbar} + A\frac{p'}{\hbar} = 0 \to \frac{A'}{A} = -\frac{1}{2}\frac{p'}{p} \to (\ln A)' = -\frac{1}{2}(\ln p)' \to A = \frac{1}{\sqrt{p}}$$

Putting it all together: $\psi(x) = \frac{1}{\sqrt{p}} e^{\pm \frac{1}{\hbar} \int p dx}$

Part c)

Problem Statement:

The classical turning points are the points where $V(x) = E$*, which implies* $p(x) = 0$*. Explain why the WKB approximation will fail near the classical turning points.*

Solution:

The WKB approximation for a wavefunction is given by:

$$\psi(x) \approx \frac{A}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int p(x') dx'},$$

where $p(x) = \sqrt{2m(E - V(x))}$ is the classical momentum of the particle and E is the total energy. Classical turning points occur where $V(x) = E$, and hence $p(x) = 0$.

The WKB approximation fails near these turning points for the following reasons:

1. Wavefunction Singularity

In the WKB approximation, the wavefunction contains the factor $\frac{1}{\sqrt{p(x)}}$. As the classical momentum $p(x)$ approaches zero near the turning point, this factor tends to infinity. This leads to a singularity in the WKB wavefunction at the turning point:

$$p(x) = \sqrt{2m(E - V(x))} \to 0 \quad \text{as} \quad V(x) \to E.$$

Therefore, the WKB approximation breaks down near the turning point because the wavefunction becomes unphysically infinite, violating the requirement that the wavefunction must remain finite everywhere.

2. Breakdown of Slowly Varying Assumption

The WKB approximation assumes that the potential $V(x)$ varies slowly relative to the wavelength of the particle. The wavelength is given by:

$$\lambda(x) = \frac{h}{p(x)}.$$

Near the turning point, where $p(x) \to 0$, the wavelength $\lambda(x)$ becomes very large (tends to infinity). This violates the basic assumption of the WKB approximation, which requires the potential $V(x)$ to change slowly on the scale of the wavelength. Thus, as $x \to x_0$, the turning point, this assumption no longer holds and the WKB approximation is no longer valid.

Part d)

Problem Statement:

Assume the potential is increasing near $x = 0$, so that $V'(0) > 0$. Show that the general solution far from $x = 0$ is of the form:

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

Solution:

Finding a solution requires us to split the wave function into x¿0 and x¡0, the reason for this is that p will become imaginary for some values. Assuming that $V'(0) > 0$ we get the following solutions.

$x > 0$

Here $V(x) > E$ since x is past the turning-point and its derivative is increasing, this means that

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

Given the general solution

$$\psi(x) = \frac{1}{\sqrt{p(x)}} \left(D e^{\frac{i}{\hbar}\int p(x')dx'} + E e^{-\frac{i}{\hbar}\int p(x')dx'} \right) = \frac{1}{\sqrt{|p(x)|}} \left(D e^{\frac{-1}{\hbar}\int_0^x |p(x')|dx'} + E e^{\frac{1}{\hbar}\int_0^x |p(x')|dx'} \right)$$

The second term will diverge as $x \to \infty$, meaning that $E = 0$, we are then left with

$$\psi(x) = \frac{1}{\sqrt{|p(x)|}} \left(D e^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'} \right)$$

$x < 0$

$p(x)$ is not imaginary here since we are not passed the turningpoint, thus we simply get with no further simplification

$$\psi(x) = \frac{1}{\sqrt{p(x)}} \left(D e^{\frac{i}{\hbar}\int p(x')dx'} + E e^{-\frac{i}{\hbar}\int p(x')dx'} \right)$$

Part e)

Problem Statement:

To find an approximate wavefunction near the turning points, we can approximate the potential as linear near $x = 0$, so that $V(x) \approx E + V'(0)x$. Defining:

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

show that the Schrödinger equation becomes:

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

Here, $\psi_p(x)$ is an approximation to the true wavefunction that is accurate near the turning point at $x = 0$. **Solution:**

Having defined

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

The partial derivative in the Schrödinger equation becomes

$$\frac{\partial^2}{\partial x^2} = \left(\frac{\partial z}{\partial x}\right)^2 \frac{\partial^2}{\partial z^2} = \alpha^2 \frac{\partial^2}{\partial z^2}$$

If we now also assume that we are close to the turningpoint: $V(x) \approx E + V'(0)x$, we get:

$$\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = (E - V(x))\,\psi(x) \Rightarrow \frac{\hbar^2}{2m}\alpha^2\frac{\partial^2}{\partial z^2}\psi(x) = -V'(0)x\ \psi(x) \rightarrow$$
$$\alpha^2\frac{\partial^2}{\partial z^2}\psi(z) = -\frac{2mV'(0)}{\hbar^2}x\psi(x) = -\alpha^3 x\psi(x) \rightarrow \frac{\partial^2}{\partial z^2}\psi_p(z) = -z\psi_p(z)$$

Part f)

Problem Statement:

Look up information on the Airy functions and find the asymptotic forms for large z.

Solution:

I found these Airy functions at DLMF[1]. In the site, they are expressed with a sum on the form:

$$\sum_{k=0}^{\infty}(-1)^k\frac{u_k}{\zeta^k}$$

All contributions here go to zero when $z \to \infty$ except the zeroth term which is equal to one, since $\zeta \propto z^{\frac{3}{2}}$. as $z \to \infty$ $(z > 0)$ I thus write:

$$\mathrm{Ai}(z) \simeq \frac{1}{2\sqrt{\pi}}|z|^{-1/4}\exp\left(-\frac{2}{3}|z|^{3/2}\right),$$

$$\mathrm{Bi}(z) \simeq \frac{e^{\frac{2}{3}|z|^{3/2}}}{\sqrt{\pi}z^{1/4}},$$

And as $z \to -\infty$ ($z < 0$):

$$\mathrm{Ai}(-z) \simeq \frac{1}{\sqrt{\pi}}|z|^{-1/4}\sin\left(\frac{2}{3}|z|^{3/2}+\frac{\pi}{4}\right)$$

$$\mathrm{Bi}(-z) \simeq \frac{1}{\sqrt{\pi}}|z|^{-1/4}\cos\left(\frac{2}{3}|z|^{3/2}+\frac{\pi}{4}\right)$$

Part g)

Problem Statement:

Show that the two solutions from part (d) and part (e) match if:

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

Solution:

We will now match the solutions in task d) with the Airy functions from f) with corresponding solution $\psi_p = aAi(\alpha x) + bBi(\alpha x)$. It can be immediately seen in task f) that if $x \to \infty$ the $Bi(z)$ function diverges to ∞, therefore b=0 in that region. For $x < 0$, both $Bi(z)$ and $Ai(z)$ take the same form, therefore both can be applied, we will however choose $Ai(z)$ here as well, for simplicity. We let $b = 0$ for both regions. We start with $x > 0$:

$$\frac{1}{\sqrt{|p(x)|}}De^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'} = \frac{a}{2\sqrt{\pi}}|z|^{-1/4}\exp\left(-\frac{2}{3}|z|^{3/2}\right),$$

Immediately, we see that:

$$\frac{1}{\hbar}\int |p(x')|dx' = \frac{2}{3}|z|^{3/2} \to p(x) = \hbar\alpha^{\frac{3}{2}}x^{\frac{1}{2}} = \hbar\alpha z^{\frac{1}{2}}$$

Which gives us

$$\frac{1}{\sqrt{\hbar\alpha}}|z|^{\frac{1}{4}}De^{-\frac{2}{3}|z|^{3/2}} = \frac{a}{2\sqrt{\pi}}|z|^{-1/4}\exp\left(-\frac{2}{3}|z|^{3/2}\right),$$

meaning that we get:

$$a = \sqrt{\frac{4\pi}{\hbar\alpha}}D$$

The matching for $x < 0$ becomes as follows

$$\frac{1}{\sqrt{p(x)}}\left(Be^{\frac{i}{\hbar}\int p(x')dx'} + Ce^{-\frac{i}{\hbar}\int p(x')dx'}\right) = \frac{a}{\sqrt{\pi}}|z|^{-1/4}\sin\left(\frac{2}{3}|z|^{3/2}+\frac{\pi}{4}\right)$$

$$\frac{1}{\sqrt{p(x)}}\left((B+C)\cos\left(\frac{1}{\hbar}\int p(x')dx'\right) + (B-C)i\sin\left(\frac{1}{\hbar}\int p(x')dx'\right)\right) = \frac{a}{\sqrt{\pi}}|z|^{-1/4}\sin\left(\frac{2}{3}|z|^{3/2}+\frac{\pi}{4}\right)$$

We get again:

$$\frac{1}{\hbar}\int |p(x')|dx' = \frac{2}{3}|z|^{3/2} \to p(x) = \hbar\alpha z^{\frac{1}{2}}$$

In order to reduce the terms down to sin alone, we must let $B = -C$. To simplify we multiply B with $e^{i\frac{\pi}{4}}$ and C with $e^{-i\frac{\pi}{4}}$.

$$\frac{1}{\sqrt{\hbar\alpha}}|z|^{\frac{1}{4}}2Bi\sin\left(\frac{2}{3}|z|^{3/2}+\frac{\pi}{4}\right) = \frac{a}{\sqrt{\pi}}|z|^{-1/4}\sin\left(\frac{2}{3}|z|^{3/2}+\frac{\pi}{4}\right)$$

We insert $a = \sqrt{\frac{4\pi}{\hbar\alpha}}D$ giving us

$$\frac{1}{\sqrt{\hbar\alpha}}|z|^{\frac{1}{4}}2Bi\sin\left(\frac{2}{3}|z|^{3/2}+\frac{\pi}{4}\right) = \sqrt{\frac{4\pi}{\hbar\alpha}}D\frac{1}{\sqrt{\pi}}|z|^{-1/4}\sin\left(\frac{2}{3}|z|^{3/2}+\frac{\pi}{4}\right)$$

Given in the current form, we get $B = -iD$ and $C = iD$, and we remember the multiplication we did prior:

$$B = -ie^{i\frac{\pi}{4}}D, \qquad C = ie^{-i\frac{\pi}{4}}D$$

This shows that the WKB solution matches the Airy functions given these parameters, which reduces the singularity issues with the general WKB solution.

Part h)

Problem Statement:

Repeat the matching procedure for a turning point where $V'(x) < 0$. Show that for a potential with a minimum, we can have bound states with energy E if:

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

Solution:

Given that $V' < 0$ means that the turning point is surpassed at $x < 0$ instead of $x > 0$, which gives imaginary $p(x) = i|p(x)|$. Thus the solution for this system is exactly the same, except that we switch the solution for $x > 0$ with $x < 0$. We can however, develop the solution further since we are given

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

The condition essentially says that the particles can only take discreete momenta between x_1 and x_2. Since the integral depends on E, we can define various E_n which satisfies the condition. We know this because $V(x)$ has a minima, which acts as a potential well with two turning points: x_1 and x_2, where $E < V(x)$, which defines bound conditions.

Part i)

Problem Statement:

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

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

Solution:

The energy eigenvalues for the harmonic oscillator can be derived as follows.

We start with the integral for the phase space area enclosed by the classical trajectory:

$$\int_{x_1}^{x_2} p(x')dx' = \left(n + \frac{1}{2}\right)\hbar, \quad \text{(Classically allowed region)}$$

Substitute $p = \sqrt{2m(E - V(x))}$ into the integral. The limits of the integration go from $-x_t$ to x_t, where $x_t = \sqrt{\frac{2E}{m\omega^2}}$ is the classical turning point. We define $\omega = \sqrt{\frac{k}{m}}$ Therefore, the integral becomes:

$$2\int_0^{x_t} \sqrt{2m\left(E - \frac{1}{2}m\omega^2 x^2\right)}\, dx = 2\int_0^{x_t} \sqrt{mk\left(x_t - x^2\right)}\, dx$$

Using the trigonometric substitution $x = x_t \sin\theta$, we have:

$$dx = x_t \cos\theta\, d\theta,$$

Since $x \in [0, x_t] \to \theta \in [0, \frac{\pi}{2}]$ and the integral becomes:

$$2\int_0^{\frac{\pi}{2}} \sqrt{mkx_t^2\left(1 - \sin^2\theta\right)} x_t \cos\theta\, d\theta = 2\int_0^{\frac{\pi}{2}} \sqrt{mk} x_t^2 \cos^2\theta\, d\theta = 2\sqrt{mk} x_t^2 \frac{\pi}{4}$$

Simplifying the terms inside the square root:

The integral $\int_0^{\frac{\pi}{2}} \cos^2\theta\, d\theta = \frac{\pi}{4}$, so:

$$= 2\sqrt{mk} x_t^2 \frac{\pi}{4} = \sqrt{mk}\frac{2E}{k}\frac{\pi}{2} = \frac{E\pi}{\omega}$$

Equating this result with $\left(n + \frac{1}{2}\right)\hbar$, we find:

$$\frac{\pi E}{\omega} = \left(n + \frac{1}{2}\right)\hbar$$

Solving for E, we get the energy eigenvalues:

$$E = \left(n + \frac{1}{2}\right)\hbar\omega.$$

Thus, the energy eigenvalues for the harmonic oscillator are quantized, with the form:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega.$$

Part j)

Problem Statement: *For the harmonic oscillator, plot the WKB wavefunctions in the various regions for one or more energy eigenstates. Include the exact eigenfunction for comparison. Select parameters to illustrate the nature of the solution clearly.* **Solution:**

The code for this can be found In the figure we see that the WKB approximation works

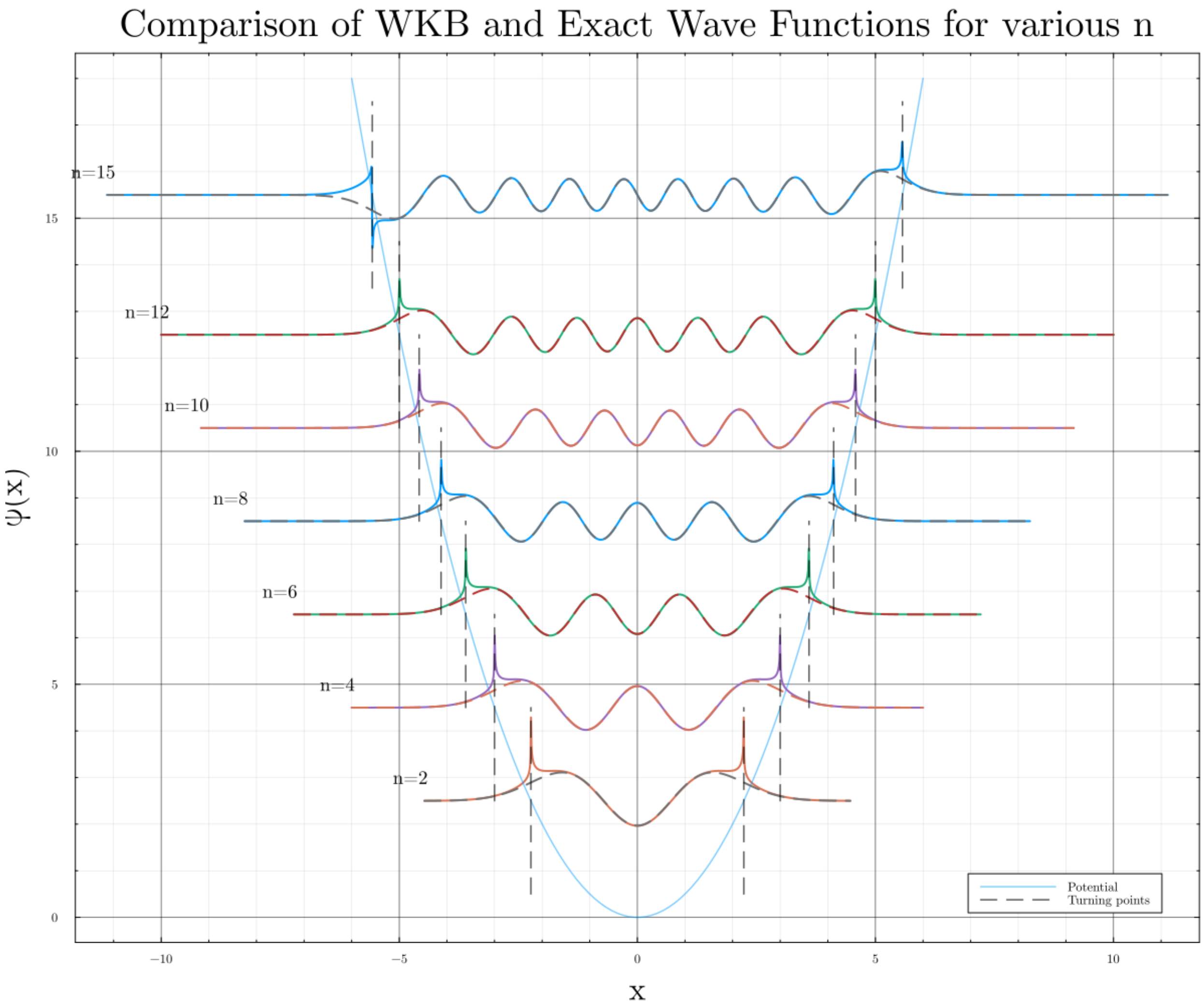

Figure 1: WKB solution for the harmonic oscillator compared to the exact solution

very well, and diverges only slightly from the analytical solutions at the turning-points. The code can be found here [2] under FYS4110.

Task 2: Semiclassical Approximation to the Path Integral

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 the action is given by:

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

The classical solution $x_c(t)$ is the one for which 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 $y(t_i) = y(t_f) = 0$.

Part a)

Problem Statement: *Show that:*

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

Solution:

We begin by expanding the action $S[x(t)]$ around the classical path $x_c(t)$ up to second order in $y(t)$.

The action is:

$$S[x(t)] = \int_{t_i}^{t_f} dt \left[\frac{1}{2}m(\dot{x}_c + \dot{y})^2 - V(x_c + y)\right].$$

Expand the kinetic and potential terms:

$$\frac{1}{2}m(\dot{x}_c + \dot{y})^2 = \frac{1}{2}m\dot{x}_c^2 + m\dot{x}_c\dot{y} + \frac{1}{2}m\dot{y}^2,$$
$$V(x_c + y) = V(x_c) + V'(x_c)y + \frac{1}{2}V''(x_c)y^2 + \frac{1}{6}V'''(x_c)y^3 + \cdots.$$

Substituting back into the action:

$$S[x(t)] = \int_{t_i}^{t_f} dt \left[\frac{1}{2}m\dot{x}_c^2 - V(x_c) + m\dot{x}_c\dot{y} - V'(x_c)y + \frac{1}{2}m\dot{y}^2 - \frac{1}{2}V''(x_c)y^2 - \frac{1}{6}V'''(x_c)y^3 + \cdots\right].$$

The action evaluated along the classical path is:

$$S[x_c] = \int_{t_i}^{t_f} dt \left[\frac{1}{2}m\dot{x}_c^2 - V(x_c)\right].$$

Therefore, the difference $\Delta S = S[x(t)] - S[x_c]$ is:

$$\Delta S = \int_{t_i}^{t_f} dt \left[m\dot{x}_c\dot{y} + \frac{1}{2}m\dot{y}^2 - V'(x_c)y - \frac{1}{2}V''(x_c)y^2 - \frac{1}{6}V'''(x_c)y^3 + \cdots\right].$$

Since $x_c(t)$ satisfies the Euler-Lagrange equation:

$$m\ddot{x}_c - V'(x_c) = 0,$$

we can integrate by parts:

$$\int_{t_i}^{t_f} m\dot{x}_c\dot{y}\, dt = -\int_{t_i}^{t_f} m\ddot{x}_c y\, dt + [m\dot{x}_c y]_{t_i}^{t_f} = -\int_{t_i}^{t_f} (V'(x_c))\, y\, dt,$$

where the boundary term vanishes due to $y(t_i) = y(t_f) = 0$.

Thus, the terms involving $V'(x_c)y$ cancel out:

$$m\dot{x}_c\dot{y} - V'(x_c)y = 0.$$

Therefore, we have:

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

Part b)

Problem Statement: *Show that the semiclassical approximation to the propagator is:*

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

Solution:

From part (a), we have expanded the action up to quadratic terms in $y(t)$:

$$S[x(t)] = S[x_c] + \int_{t_i}^{t_f} dt\left[\frac{1}{2}m\dot{y}^2 - \frac{1}{2}V''(x_c)y^2\right].$$

The path integral becomes:

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

In the semiclassical approximation, we neglect the higher-order terms in y. Therefore:

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

Part c)

Problem Statement: *Check that the propagator in the equation above corresponds to the known propagators for the free particle and the harmonic oscillator for specific choices of $W(x)$ and the function $f(t)$.* **Solution:**

Free Particle ($V(x) = 0$):

A free particle is a particle under no influence, including any potential. V(x) is thus set to 0. This means that W(x) is also set to zero. We choose $f(t)$:

$$\frac{\partial^2}{\partial x^2} f(t) = 0 \rightarrow f(t) = at + b$$

It is thus a straight line. We will simply choose $f(t) = t$ and we use

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

And we Evaluate the integral

$$\int_{t_i}^{t_f}\frac{dt}{f^2(t)} = \int_{t_i}^{t_f}\frac{dt}{t^2} = \frac{1}{t_i} - \frac{1}{t_f}$$

Considering that we also have the terms $f(t_i)f(t_f) = t_i t_f$ we get

$$\frac{t_i t_f}{t_i} - \frac{t_i t_f}{t_f} = t_f - t_i$$

$$\sqrt{\frac{m}{2\pi i\hbar f(t_i)f(t_f)\int_{t_i}^{t_f}\frac{dt}{f^2(t)}}} = \sqrt{\frac{m}{2\pi i\hbar(t_f-t_i)}}$$

We must now evaluate the exponential

$$e^{\frac{i}{\hbar}S[x_c]} = e^{\frac{i}{\hbar}\int_{t_i}^{t_f}dt\frac{1}{2}m\dot{x}_c^2}$$

In order to solve the integral, we consider that x_c corresponds to a classical path, which in this case is simply a straight line:

$$\int_{t_i}^{t_f}dt\frac{1}{2}m\left(\frac{d}{dt}\left(x_i+\frac{x_f-x_i}{t_f-t_i}t\right)\right)^2) = \int_{t_i}^{t_f}dt\frac{1}{2}m\left(\frac{x_f-x_i}{t_f-t_i}\right)^2 = \frac{1}{2}m\frac{(x_f-x_i)^2}{t_f-t_i}$$

Meaning that we get

$$G(x_f,t_f;x_i,t_i) = e^{\frac{i}{\hbar}S[x_c]}\sqrt{\frac{m}{2\pi i\hbar(t_f-t_i)}} = e^{\frac{im(x_f-x_i)^2}{2\hbar(t_f-t_i)}}\sqrt{\frac{m}{2\pi i\hbar(t_f-t_i)}}$$

Which is indeed the propagator for a free particle.

Harmonic Oscillator $(V(x)=\frac{1}{2}m\omega^2x^2)$

For the harmonic oscillator, we set $W=\frac{1}{m}V''(x_c)=\omega^2$. Thus we must solve

$$\frac{\partial^2}{\partial x^2}f(t) = -w^2f(t) \to f(t) = Ae^{iwt}+Be^{-iwt}$$

We must choose A and B, we know that for a harmonic oscillator, we should get:

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

Meaning that $f(t_i)f(t_f)\int_{t_i}^{t_f}\frac{1}{f(t)^2} = \frac{\sin(\omega(t_f-t_i))}{\omega}$. Thus we try $A=\frac{1}{2}, B=\frac{1}{2}\to f(t)=cos(\omega t)$ and evaluate:

$$f(t_i)f(t_f)\int_{t_i}^{t_f}\frac{1}{f(t)^2} = \cos(\omega t_i)\cos(\omega t_f)\int_{t_i}^{t_f}\frac{1}{\cos(\omega t)^2} = \cos(\omega t_i)\cos(\omega t_f)\frac{1}{\omega}\left(\tan(\omega t_f)-\tan(\omega t_i)\right)$$

$$= \frac{1}{\omega}(\sin(\omega t_f)\cos(\omega t_i)-\sin(\omega t_i)\cos(\omega t_f)) = \frac{1}{\omega}\sin(\omega(t_f-t_i))$$

Now, again, we must evaluate the exponential.

$$e^{\frac{i}{\hbar}S[x_c]} = e^{\frac{i}{\hbar}\int_{t_i}^{t_f}dt\frac{1}{2}m\dot{x}_c^2+\frac{1}{2}kx^2}$$

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

The general solution for the classical harmonic oscillator is:

$$x_c(t) = A\cos(\omega t)+B\sin(\omega t),$$

where A and B are determined by the boundary conditions $x(t_i) = x_i$ and $x(t_f) = x_f$. Applying these conditions, we express the solution as:

$$x_c(t) = \frac{x_f \sin(\omega(t - t_i)) + x_i \sin(\omega(t_f - t))}{\sin(\omega T)},$$

where $T = t_f - t_i$ is the time difference. The time derivative of $x_c(t)$ is:

$$\dot{x}_c(t) = \frac{\omega \left(x_f \cos(\omega(t - t_i)) - x_i \cos(\omega(t_f - t))\right)}{\sin(\omega T)}.$$

Now, we substitute $x_c(t)$ and $\dot{x}_c(t)$ into the classical action:

$$S_{\text{cl}} = \int_{t_i}^{t_f} \left(\frac{1}{2} m \dot{x}_c^2 - \frac{1}{2} m \omega^2 x_c^2 \right) dt.$$

Kinetic Energy Term:

$$T = \frac{1}{2} m \dot{x}_c^2 = \frac{1}{2} m \left(\frac{\omega \left(x_f \cos(\omega(t - t_i)) - x_i \cos(\omega(t_f - t))\right)}{\sin(\omega T)} \right)^2.$$

Potential Energy Term:

$$V = \frac{1}{2} m \omega^2 x_c^2 = \frac{1}{2} m \omega^2 \left(\frac{x_f \sin(\omega(t - t_i)) + x_i \sin(\omega(t_f - t))}{\sin(\omega T)} \right)^2.$$

The integral of the kinetic and potential energy terms gives the classical action:

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

We are left with the exponential

$$\exp\left(\frac{i}{\hbar} S_{\text{cl}} \right) = \exp\left(\frac{i m \omega}{2 \hbar \sin(\omega T)} \left[(x_f^2 + x_i^2) \cos(\omega T) - 2 x_f x_i \right] \right).$$

Thus, the full propagator for the harmonic oscillator is:

$$G(x_f, t_f; x_i, t_i) = \sqrt{\frac{m\omega}{2\pi i \hbar \sin(\omega T)}} \exp\left(\frac{i m \omega}{2 \hbar \sin(\omega T)} \left[(x_f^2 + x_i^2) \cos(\omega T) - 2 x_f x_i \right] \right).$$

This matches the known propagator for the harmonic oscillator.

Therefore, the semiclassical approximation recovers the known propagators for these systems.

Part d)

Problem Statement: *Show that:*

$$G(T) = \sum_n e^{-\frac{i}{\hbar}E_n T}, \quad \text{and} \quad G(E) = \sum_n \frac{1}{E_n - E}.$$

Solution:

We have $G(T)$

$$G(T) = \int_{-\infty}^{\infty} G(x, T; x, 0)\, dx.$$

Expressed in terms of eigenstates:

$$G(x, T; x, 0) = \sum_n \psi_n(x)\psi_n^*(x) e^{-\frac{i}{\hbar}E_n T}.$$

Here, $\psi_n(x)$ are the energy eigenfunctions satisfying $\hat{H}\psi_n(x) = E_n\psi_n(x).G(T)$ is:

$$G(T) = \int_{-\infty}^{\infty} \left(\sum_n \psi_n(x)\psi_n^*(x) e^{-\frac{i}{\hbar}E_n T} \right) dx = \sum_n e^{-\frac{i}{\hbar}E_n T} \int_{-\infty}^{\infty} |\psi_n(x)|^2 dx.$$

Where we use:

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1.$$

Therefore:

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

Computing $G(E)$:

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

The integral converges if we introduce an infinitesimal positive imaginary part to E:

$$\int_0^{\infty} e^{\frac{i}{\hbar}(E - E_n + i\epsilon)T} dT = \frac{\hbar}{E_n - E - i\epsilon}.$$

Taking $\epsilon \to 0^+$, we get:

$$\frac{i}{\hbar} \int_0^{\infty} e^{\frac{i}{\hbar}(E - E_n)T} dT = \frac{1}{E_n - E}.$$

Therefore:

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

Part e)

Problem Statement: *Apply equations (8) and (10) to the harmonic oscillator and check that they give the correct energy levels.* **Solution:**

$$G(x_0, T; x_0, 0) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}} \exp\left(\frac{im\omega x_0^2(\cos(\omega T) - 1)}{\hbar \sin(\omega T)}\right).$$

We now compute the integral:

$$I = \int_{-\infty}^{\infty} G(x_0, T; x_0, 0)\, dx_0.$$

This becomes:

$$I = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}} \int_{-\infty}^{\infty} \exp\left(\frac{im\omega x_0^2(\cos(\omega T) - 1)}{\hbar \sin(\omega T)}\right) dx_0.$$

The Gaussian integral is:

$$\int_{-\infty}^{\infty} \exp(ax_0^2)\, dx_0 = \sqrt{\frac{\pi}{-a}},$$

with:

$$a = \frac{im\omega(\cos(\omega T) - 1)}{\hbar \sin(\omega T)}.$$

We get after simpifying

$$G(T) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}}\sqrt{\frac{\pi\hbar \sin(\omega T)}{-im\omega(\cos(\omega T) - 1)}} = \sqrt{\frac{1}{-2(\cos(\omega T) - 1)}} = \frac{1}{2i\sin(\omega T/2)}$$

We now show that we get the same from the expression from part (d), where we have:

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

For the harmonic oscillator, the energy levels are:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots$$

$G(T)$ for the harmonic oscillator is given by:

$$G(T) = \sum_{n=0}^{\infty} e^{-i\omega\left(n+\frac{1}{2}\right)T}.$$

This is a geometric series with:

$$q = e^{-i\omega T}.$$

Then:

$$G(T) = e^{-i\frac{\omega T}{2}} \sum_{n=0}^{\infty} q^n = e^{-i\frac{\omega T}{2}}\left(\frac{1}{1-q}\right), \quad \text{if } |q| < 1.$$

We now evaluate

$$G(T) = e^{-i\frac{\omega T}{2}} \frac{1}{1 - e^{-i\omega T}} = \frac{1}{e^{i\frac{\omega T}{2}} - e^{-i\frac{\omega T}{2}}} = \frac{1}{2i\sin(\omega\frac{T}{2})}$$

Thus we get the correct energy levels for the harmonic oscillator.

Part f)

Problem Statement: *Using equation (7) from the problem set, show that in this case we can choose $f(t) = \dot{x}_c(t)$, and derive that:*

$$G(T) = \int dx_0 \, e^{\frac{i}{\hbar}S[x_c]} \sqrt{\frac{m}{2\pi i\hbar \dot{x}_c(0)\dot{x}_c(T)}} \left(\int_0^T \frac{dt}{\dot{x}_c^2(t)} \right)^{-1/2}.$$

Solution:

We start the solution by evaluation the classical Lagrangian for the system:

$$L = \frac{1}{2}m\dot{x}_c^2 - V(x_c).$$

The classical equation of motion is obtained from the Euler-Lagrange equation:

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

Let's compute each term. First, the derivative of the Lagrangian with respect to the velocity $\dot{x}_c$:

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

Taking the time derivative gives:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_c}\right) = m\ddot{x}_c.$$

Next, the derivative of the Lagrangian with respect to the position x_c:

$$\frac{\partial L}{\partial x_c} = -V'(x_c).$$

Thus, the Euler-Lagrange equation becomes the classical equation of motion:

$$m\ddot{x}_c + V'(x_c) = 0.$$

This is the equation of motion for the classical path $x_c(t)$. We are given the differential equation:

$$\frac{d^2}{dt^2}f(t) + W(t)f(t) = 0,$$

where $W(t) = V''(x_c(t))$. We choose $f(t) = \dot{x}_c(t)$, and we want to show that this function satisfies the differential equation. The first derivative of $f(t)$ is:

$$\frac{d}{dt}f(t) = \ddot{x}_c(t).$$

Taking the second derivative:

$$\frac{d^2}{dt^2}f(t) = \frac{d}{dt}\ddot{x}_c(t).$$

From the classical equation of motion, we know:

$$\ddot{x}_c(t) = -\frac{1}{m} V'(x_c(t)).$$

Taking the time derivative of this equation:

$$\frac{d}{dt}\ddot{x}_c(t) = -\frac{1}{m} V''(x_c(t))\dot{x}_c(t).$$

Thus, the second derivative of $f(t)$ is:

$$\frac{d^2}{dt^2} f(t) = -\frac{1}{m} V''(x_c(t))\dot{x}_c(t).$$

Since $W(t) = V''(x_c(t))$, we see that:

$$\frac{d^2}{dt^2} f(t) + W(t) f(t) = 0.$$

This confirms that $f(t) = \dot{x}_c(t)$ satisfies the differential equation. We now put everything together and get that the semiclassical approximation to the propagator is given by:

$$G(T) = \int dx_0 e^{\frac{i}{\hbar} S[x_c]} \sqrt{\frac{m}{2\pi i \hbar \dot{x}_c(0) \dot{x}_c(T)}} \left(\int_0^T \frac{dt}{\dot{x}_c^2(t)} \right)^{-1/2}.$$

By choosing $f(t) = \dot{x}_c(t)$, we satisfy the differential equation and obtain the correct form for the propagator in the semiclassical approximation.

Part g)

Problem Statement: *Show that these are the periodic solutions* The integral under consideration is:

$$G(T) = \int dx_0 \, e^{\frac{i}{\hbar} S[x_c]} \sqrt{\frac{m}{2\pi i \hbar \dot{x}_c(0) \dot{x}_c(T)}} \left[\int_0^T dt \, \dot{x}_c^2(t) \right]^{-\frac{1}{2}}$$

Solution:

In the semiclassical limit, $\hbar \to 0$, the integral over x_0 is dominated by points where the phase is stationary with respect to x_0. This condition is expressed as:

$$\frac{d}{dx_0} \left(\frac{1}{\hbar} S[x_c] \right) = 0 \quad \Rightarrow \quad \frac{dS}{dx_0} = 0$$

The total derivative of S with respect to x_0 is:

$$\frac{dS}{dx_0} = \frac{\partial S}{\partial x_i} + \frac{\partial S}{\partial x_f} \frac{dx_f}{dx_0}$$

From classical mechanics, we know:

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

Therefore:

$$\frac{dS}{dx_0} = -p_i + p_f \frac{dx_f}{dx_0}$$

For the classical trajectory $x_c(t)$, x_f depends on x_0. To understand this relationship, we consider the derivative $\frac{dx_f}{dx_0}$. For periodic solutions, where the particle returns to its starting point after time T:

$$x_f = x_0 \quad \Rightarrow \quad \frac{dx_f}{dx_0} = 1$$

Substituting $\frac{dx_f}{dx_0} = 1$ into the expression for $\frac{dS}{dx_0}$ gives:

$$\frac{dS}{dx_0} = -p_i + p_f$$

Setting $\frac{dS}{dx_0} = 0$ leads to the condition:

$$-p_i + p_f = 0 \quad \Rightarrow \quad p_i = p_f$$

The condition $p_i = p_f$ implies that the particle has the same momentum at $t = 0$ and $t = T$. Along with $x_f = x_0$, this means the particle returns to its initial position with the same momentum after time T. This is the defining feature of a periodic solution.

To validate the results, we account for the pre-factor term as well, arguing that it does not induce rapid oscillations at periodic solutions. The integral $G(T)$ also contains a pre-factor involving $\dot{x}_c(0)$, $\dot{x}_c(T)$, and an integral over $\dot{x}_c^2(t)$:

$$\text{Pre-factor} = \sqrt{\frac{m}{2\pi i\hbar \dot{x}_c(0)\dot{x}_c(T)}} \left[\int_0^T dt\, \dot{x}_c^2(t)\right]^{-\frac{1}{2}}$$

For Periodic Solutions, $x_f = x_0$ and $p_f = p_i$, the velocities at $t = 0$ and $t = T$ are equal:

$$\dot{x}_c(T) = \dot{x}_c(0)$$

Thus, the product simplifies:

$$\dot{x}_c(0)\dot{x}_c(T) = [\dot{x}_c(0)]^2$$

The pre-factor becomes:

$$\sqrt{\frac{m}{2\pi i\hbar \left[\dot{x}_c(0)\right]^2}} \left[\int_0^T dt\, \dot{x}_c^2(t)\right]^{-\frac{1}{2}}$$

This pre-factor is a smooth function of x_0 and does not introduce any rapid oscillations.

For non-periodic solutions, where $x_f \neq x_0$ and $p_f \neq p_i$, the phase $e^{\frac{i}{\hbar}S[x_c]}$ oscillates rapidly as x_0 varies, causing these contributions to cancel out upon integration. We have found that the integral $G(T)$ is dominated by contributions from periodic solutions, where $\frac{dS}{dx_0} = 0$. Non-periodic solutions contribute negligibly due to destructive interference from the rapidly oscillating phase. The pre-factor does not alter this conclusion, hence, $G(T)$ is predominantly determined by periodic solutions.

Part h)

Problem Statement:

Explain why both $S_{T/n}$ and $\int_0^T \frac{dt}{\dot{x}^2_{T/n}(t)}$ are independent of x_0, and show that:

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

Solution:

1. Independence of $S_{T/n}$ on x_0:

- $S_{T/n}$ represents the action evaluated along the classical solution $x_{T/n}(t)$ over the time interval T. - For periodic systems (like the harmonic oscillator), the action over a full period is independent of the initial position x_0.

This is because the action $S_{T/n}$ depends on the energy of the system. In periodic systems, the energy is constant along the motion. Qnd since the energy is determined by the amplitude (which can be related to x_0 but cycles through all possible values over a period), the action becomes independent of x_0.

2. Independence of $\int_0^T \frac{dt}{\dot{x}^2_{T/n}(t)}$ on x_0:

- This integral averages $\frac{1}{\dot{x}^2_{T/n}(t)}$ over the time interval T. The function $\dot{x}_{T/n}(t)$ is periodic. When integrated over a full period, any dependence on the initial phase (determined by x_0) cancels out. Thus, the integral depends only on the properties of the periodic motion, not on x_0.

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

Since $x_{T/n}(t)$ is a periodic function with period $T_{\text{cl}} = \frac{T}{n}$, the initial position $x_0 = x_{T/n}(0)$ varies as t varies over one period.

I Use the inverse function theorem:

Consider $x_0 = x_{T/n}(t)$. Then, $dx_0 = \dot{x}_{T/n}(t)dt$. Therefore:

$$dt = \frac{dx_0}{\dot{x}_{T/n}(t)}.$$

Since $\dot{x}_{T/n}(t)$ can be positive or negative depending on t, we take the absolute value to ensure positive integration measures:

$$dt = \frac{dx_0}{|\dot{x}_{T/n}(t)|}.$$

When we integrate both sides over one period:

$$\int_{x_{\min}}^{x_{\max}} \frac{1}{|\dot{x}_{T/n}(0)|} dx_0 = \int_0^{T_{\text{cl}}} dt = \frac{T}{n}.$$

Therefore, we have shown that:

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

Part i)

Problem Statement:

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

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

Solution:

From previous parts (specifically parts (f) and (g)), we have an expression for the propagator $G(T)$:

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

We are given that:

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

Let $T = nu$, so $dT = ndu$. Substituting into $G(E)$:

$$G(E) = \frac{i}{\hbar}\sum_{n=1}^{\infty}\int dx_0 \int_0^{\infty} ndu\, e^{\frac{i}{\hbar}nS_u} e^{\frac{i}{\hbar}nEu} \frac{m}{2\pi i\hbar}\frac{1}{|\dot{x}_u(0)|}\left[\int_0^{nu} dt\, \dot{x}^2_u(t)\right]^{-1/2}.$$

Since $\dot{x}_u(t)$ is periodic with period u, the integral over t becomes:

$$\int_0^{nu} dt\, \dot{x}^2_u(t) = n\int_0^u dt\, \dot{x}^2_u(t).$$

Thus, the expression simplifies to:

$$G(E) = \frac{i}{\hbar}\sum_{n=1}^{\infty}\int dx_0 \int_0^{\infty} du\, e^{\frac{i}{\hbar}n(Eu+S_u)} n \frac{m}{2\pi i\hbar}\frac{1}{|\dot{x}_u(0)|}\left[\int_0^{u} dt\, \dot{x}^2_u(t)\right]^{-1/2}.$$

From part (h), we have:

$$\int dx_0 \frac{1}{|\dot{x}_u(0)|} = u.$$

Assuming $\dot{x}_u(0)$ depends on x_0, integrating over x_0 yields:

$$\int dx_0 \left(\frac{1}{|\dot{x}_u(0)|}\right)^{1/2} = u.$$

We use the following relation:

$$\left[\int_0^u dt\, \dot{x}^2_u(t)\right]^{-1} = \frac{dE_u}{du}.$$

This follows from the relation between time and energy in classical mechanics. Substituting the above results, we have:

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

Part j)

Problem Statement:

Use the stationary phase approximation with $\frac{1}{\hbar}$ as the large parameter and show that:

$$G(E) = \frac{i}{\hbar}\sum_{n=1}^{\infty}(-1)^n e^{\frac{i}{\hbar}nW_{u_0}},$$

where $u_0(E)$ is found as the solution of $E - E_{u_0} = 0$, and $W = S_{u_0} + Eu_0$.

Solution: From part (i), we have:

$$G(E) = \frac{i}{\hbar}\frac{i}{2\pi\hbar}\sum_{n=1}^{\infty}(-1)^n n \int_0^{\infty} du\, e^{\frac{i}{\hbar}n\Phi(u)} \left(\frac{dE_u}{du}\right)^{1/2},$$

where:

$$\Phi(u) = Eu + S_u.$$

We apply the Stationary Phase Approximation:

We consider $\hbar$ to be small, so $\frac{1}{\hbar}$ is large. For each n, the phase is $n\Phi(u)$. Set the derivative of the phase to zero:

$$\frac{d}{du}(n\Phi(u)) = n\Phi'(u) = 0 \quad \Rightarrow \quad \Phi'(u_0) = 0.$$

Compute $\Phi'(u)$:

$$\Phi'(u) = E + \frac{dS_u}{du} = E - E_u,$$

since $\frac{dS_u}{du} = -E_u$. Therefore, the stationary point satisfies:

$$E - E_{u_0} = 0 \quad \Rightarrow \quad E = E_{u_0}.$$

With second derivative

$$\Phi''(u) = -\frac{dE_u}{du}.$$

Using the stationary phase approximation:

$$\int_0^{\infty} du\, e^{in\Phi(u)} f(u) \approx e^{in\Phi(u_0)} f(u_0) \frac{2\pi}{n|\Phi''(u_0)|}.$$

At $u = u_0$:

$$f(u_0) = n\left(\left.\frac{dE_u}{du}\right|_{u=u_0}\right)^{1/2}.$$

The second derivative:

$$|\Phi''(u_0)| = \left|-\left.\frac{dE_u}{du}\right|_{u=u_0}\right| = \left.\frac{dE_u}{du}\right|_{u=u_0}.$$

Therefore, the integral becomes:

$$\int_0^{\infty} du\, e^{in\Phi(u)} f(u) \approx e^{in\Phi(u_0)} \frac{2\pi}{n}.$$

Including the prefactor $\frac{i}{2\pi\hbar}$, we have:

$$G(E) \approx \frac{i}{\hbar} \sum_{n=1}^{\infty} (-1)^n e^{\frac{i}{\hbar} n \Phi(u_0)}.$$

Since $\Phi(u_0) = Eu_0 + S_{u_0} = W$, we get:

$$G(E) = \frac{i}{\hbar} \sum_{n=1}^{\infty} (-1)^n e^{\frac{i}{\hbar} nW}.$$

Part k)

Problem Statement: *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:*

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

Solution:
We have:

$$G(E) = \frac{i}{\hbar} u_0 \sum_{n=1}^{\infty} (-1)^n e^{\frac{i}{\hbar} nW} = \frac{i}{\hbar} u_0 \left(-\frac{e^{\frac{i}{\hbar} W}}{1 - e^{\frac{i}{\hbar} W}} \right).$$

The poles occur when the denominator vanishes:

$$1 - e^{\frac{i}{\hbar} W} = 0 \quad \Rightarrow \quad e^{\frac{i}{\hbar} W} = 1 \quad \Rightarrow \frac{W}{\hbar} = 2\pi n.$$

We have:

$$W = S_{u_0} + Eu_0 = \text{Total action over one period.}$$

In classical mechanics, the action over one period is:

$$W = 2 \int_{x_1}^{x_2} p(x')dx',$$

where $p(x) = \sqrt{2m(E - V(x))}$ is the classical momentum. Substituting back:

$$2 \int_{x_1}^{x_2} p(x')dx' = 2\pi\hbar(n + 1/2).$$

Dividing both sides by 2:

$$\int_{x_1}^{x_2} p(x')dx' = \pi\hbar \left(n + \frac{1}{2}\right).$$

Problem 3 — Comparing the two approximations

Part a)

Problem Statement: *We write the wavefunction as:*

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

Show that $f(x)$ satisfies

$$i\hbar f''(x) - [f'(x)]^2 + p^2(x) = 0.$$

Solution: The one-dimensional time-independent Schrödinger equation is:

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

Define the classical momentum $p(x)$ as:

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

We are given:

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

With the first derivative:

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

And the second derivative:

$$\psi''(x) = \left(\frac{i}{\hbar} f'(x)\right)' \psi(x) + \left(\frac{i}{\hbar} f'(x)\right)^2 \psi'(x),$$

which simplifies to:

$$\psi''(x) = \frac{i}{\hbar} f''(x)\psi(x) - \left(\frac{f'(x)}{\hbar}\right)^2 \psi(x).$$

Substitute $\psi''(x)$ into the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\left(\frac{i}{\hbar} f''(x)\psi(x) - \left(\frac{f'(x)}{\hbar}\right)^2 \psi(x)\right) + V(x)\psi(x) = E\psi(x).$$

Simplifying the terms:

$$-\frac{\hbar^2}{2m}\left(\frac{i}{\hbar} f''(x) - \frac{f'(x)^2}{\hbar^2}\right)\psi(x) + V(x)\psi(x) = E\psi(x).$$

Divide through by $\psi(x)$ and simplify:

$$\frac{\hbar^2}{2m}\left(\frac{i}{\hbar} f''(x) - \frac{f'(x)^2}{\hbar^2}\right) + V(x) = E.$$

Bring all terms to one side:

$$-\frac{\hbar^2}{2m}\left(\frac{i}{\hbar}f''(x) - \frac{f'(x)^2}{\hbar^2}\right) + V(x) - E = 0.$$

Noting that $V(x) - E = -[E - V(x)]$, we have:

$$-\hbar^2\left(\frac{i}{\hbar}f''(x) - \frac{f'(x)^2}{\hbar^2}\right) - 2m[E - V(x)] = 0.$$

Since $p^2(x) = 2m[E - V(x)]$, we obtain:

$$i\hbar f''(x) - [f'(x)]^2 + p^2(x) = 0.$$

Part b)

Problem Statement:

Write $f(x)$ as a power series in $\hbar$:

$$f(x) = f_0(x) + \hbar f_1(x) + \hbar^2 f_2(x) + \dots.$$

Show that if we keep only terms up to first order in $\hbar$, we get the WKB wavefunctions:

$$\psi_\pm(x) = \frac{1}{\sqrt{p(x)}}e^{\pm\frac{i}{\hbar}\int p(x)\,dx}.$$

Solution:

From part (a), we have:

$$i\hbar f''(x) - [f'(x)]^2 + p^2(x) = 0.$$

Substitute $f(x) = f_0(x)+\hbar f_1(x)+\hbar^2 f_2(x)+\dots$ into the equation. Compute $f'(x)$ and $f''(x)$:

$$f'(x) = f_0'(x) + \hbar f_1'(x) + \hbar^2 f_2'(x) + \dots,$$

$$f''(x) = f_0''(x) + \hbar f_1''(x) + \hbar^2 f_2''(x) + \dots.$$

We now substitute into the equation:

$$i\hbar(f_0'' + \hbar f_1'' + \dots) - (f_0' + \hbar f_1' + \dots)^2 + p^2 = 0.$$

and expand the square:

$$(f_0' + \hbar f_1' + \dots)^2 = [f_0']^2 + 2\hbar f_0' f_1' + \hbar^2(2f_0' f_2' + [f_1']^2) + \dots.$$

Substituting back:

$$i\hbar f_0'' + i\hbar^2 f_1'' + \dots - ([f_0']^2 + 2\hbar f_0' f_1' + \dots) + p^2 = 0.$$

- Order $\hbar^0$:

$$-[f_0'(x)]^2 + p^2(x) = 0,$$

which gives:

$$[f_0'(x)]^2 = p^2(x).$$

$$i f_0''(x) - 2f_0'(x)f_1'(x) = 0.$$

Solve the Zeroth-Order Equation:

$$[f_0'(x)]^2 = p^2(x).$$

Therefore:

$$f_0'(x) = \pm p(x).$$

Integrating:

$$f_0(x) = \pm \int p(x)\, dx + C_0.$$

We can absorb C_0 into the normalization constant, so we set $C_0 = 0$. Solve the First-Order Equation:

$$i f_0''(x) - 2f_0'(x)f_1'(x) = 0.$$

Since $f_0'(x) = \pm p(x)$ and $f_0''(x) = \pm p'(x)$, the equation becomes:

$$i(\pm p'(x)) - 2(\pm p(x))f_1'(x) = 0.$$

Simplifying:

$$f_1'(x) = \frac{ip'(x)}{2p(x)}.$$

Integrating:

$$f_1(x) = \frac{i}{2} \ln p(x) + C_1.$$

Again, C_1 can be absorbed into the normalization. Up to first order in $\hbar$:

$$\psi(x) = e^{\frac{i}{\hbar} f(x)} = e^{\frac{i}{\hbar}(f_0(x) + \hbar f_1(x))} = e^{\frac{i}{\hbar} f_0(x)} e^{i f_1(x)}.$$

Substituting $f_0(x)$ and $f_1(x)$:

$$\psi(x) = e^{\pm \frac{i}{\hbar} \int p(x) dx} \cdot e^{i\left(\frac{i}{2} \ln p(x)\right)} = e^{\pm \frac{i}{\hbar} \int p(x) dx} \cdot \frac{1}{\sqrt{p(x)}}.$$

Therefore, the wavefunctions are:

$$\psi_\pm(x) = \frac{1}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int p(x)\, dx}.$$

Part c)

Problem Statement: *To see that the semiclassical approximation to the path integral can be considered the first term in an expansion in powers of $\hbar$, we revisit the expansion of the action:*

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

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

Solution:

Let:

$$z(t) = \frac{y(t)}{\hbar} \quad \Rightarrow \quad y(t) = \hbar z(t).$$

Express $\Delta S_n(y^n)$ in terms of $z(t)$:

$$\Delta S_2(y^2) = \Delta S_2(\hbar z^2),$$

$$\Delta S_3(y^3) = \Delta S_3((\hbar z)^3) = \hbar^{3/2} \Delta S_3(z^3),$$

$$\Delta S_4(y^4) = \Delta S_4((\hbar z)^4) = \hbar^2 \Delta S_4(z^4),$$

and so on.

$$S[x(t)] = S[x_c] + \hbar \Delta S_2(z^2) + \hbar^{3/2} \Delta S_3(z^3) + \hbar^2 \Delta S_4(z^4) + \dots.$$

The path integral becomes:

$$G = e^{\frac{i}{\hbar} S[x_c]} \int \mathcal{D}y(t)\, e^{\frac{i}{\hbar}\left(\Delta S_2(y^2) + \Delta S_3(y^3) + \dots\right)}.$$

Substitute $y(t) = \hbar z(t)$:

$$G = e^{\frac{i}{\hbar} S[x_c]} \int \mathcal{D}(\hbar z(t))\, e^{\frac{i}{\hbar}\left(\hbar \Delta S_2(z^2) + \hbar^{3/2} \Delta S_3(z^3) + \dots\right)}.$$

Divide both sides by $\hbar$:

$$\frac{i}{\hbar}\left(\hbar \Delta S_2(z^2) + \hbar^{3/2} \Delta S_3(z^3) + \dots\right) = i \Delta S_2(z^2) + i \hbar^{1/2} \Delta S_3(z^3) + i \hbar \Delta S_4(z^4) + \dots.$$

The second-order term $i \Delta S_2(z^2)$ is independent of $\hbar$. The third-order term $i\hbar^{1/2} \Delta S_3(z^3)$ is proportional to $\hbar^{1/2}$. The fourth-order term $i\hbar \Delta S_4(z^4)$ is proportional to $\hbar$.

As $\hbar \to 0$:

The second-order term remains finite. The third-order term and higher-order terms become negligible because they are multiplied by higher powers of $\hbar$.

Therefore, in the limit $\hbar \to 0$, the contribution of the ΔS_3 term and higher-order terms becomes small compared to the second-order term $\Delta S_2(z^2)$. This justifies the semiclassical approximation, where we keep only terms up to quadratic order in the deviations from the classical path.

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