

- (a) Show that the WKB method reproduces the exact results for the energy eigenvalues of the harmonic oscillator potential, $V(x) = \frac{1}{2}m\omega^2x^2$.
- (b) Analyze the validity criterion, $|k'(x)/k(x)^2| \ll 1$ as a function of the energy eigenstate label n .

a. Energy eigenvalues

For $V(x) = \frac{1}{2}m\omega^2x^2$, we find the classical turning point as $E = V(\pm A)$ where

$$A = \sqrt{\frac{2E}{m\omega^2}}, \quad E = \frac{A^2 m \omega^2}{2} \quad (1)$$

in the regime $E > V(x)$, define the quantum number for WKB:

$$k(x) = \frac{1}{\hbar} \sqrt{2m \left(E - \frac{1}{2}m\omega^2x^2 \right)} = \frac{m\omega}{\hbar} \sqrt{A^2 - x^2}. \quad (2)$$

Recall the WKB quantization condition for a single smooth bound state:

$$\int_{x_1}^{x_2} k(x) dx = \left(n + \frac{1}{2} \right) \pi \quad (3)$$

where $x_1 = -A$, $x_2 = A$. We compute the integral:

$$\int_{x_1}^{x_2} k(x) dx = \frac{m\omega}{\hbar} \int_{-A}^A \sqrt{A^2 - x^2} dx = \frac{m\omega \pi A^2}{\hbar 2} = \frac{\pi E}{\hbar \omega}. \quad (4)$$

Letting this equal to $\left(n + \frac{1}{2}\right)\pi$, we solve for the energy levels:

$$\frac{\pi E}{\hbar \omega} = \left(n + \frac{1}{2} \right) \pi \Rightarrow E_n = \left(n + \frac{1}{2} \right) \hbar \omega, \quad n = 0, 1, 2, \dots \quad (5)$$

exactly as expected from the quantum harmonic oscillator solution.

b. Validity Criterion

Recall the validity criterion for WKB approximation:

$$\left| \frac{k'}{k^2} \right| \ll 1. \quad (6)$$

We evaluate LHS and find the edge of the validity region. First, we have

$$k = \frac{m\omega}{\hbar} \sqrt{A^2 - x^2} \Rightarrow k' = \frac{m\omega}{\hbar} \frac{-x}{\sqrt{A^2 - x^2}}. \quad (7)$$

Then

$$\left| \frac{k'}{k^2} \right| = \left| -\frac{\hbar}{m\omega} \frac{x}{(A^2 - x^2)^{\frac{3}{2}}} \right| = l^2 \frac{|x|}{(A^2 - x^2)^{\frac{3}{2}}} \quad (8)$$

where we defined the characteristic length scale $l := \sqrt{\frac{\hbar}{m\omega}}$.

We further define a dimensionless position variable $\alpha = \frac{|x|}{A}$, where

$$A = \sqrt{\frac{2E}{m\omega^2}} = l \sqrt{2 \left(n + \frac{1}{2} \right)} \quad (9)$$

Following the non-dimensionalization, we have

$$\left| \frac{k'}{k^2} \right| = \frac{\alpha l^2}{A^2(1-\alpha^2)^{\frac{3}{2}}} = \frac{\alpha}{2(n+\frac{1}{2})(1-\alpha^2)^{\frac{3}{2}}} \quad (10)$$

We study the limit $\alpha \rightarrow 0$ and $\alpha \rightarrow 1$:

- As $\alpha \rightarrow 0$,

$$\left| \frac{k'}{k^2} \right| \sim \frac{1}{n} \quad (11)$$

and the WKB is valid for large n .

- As $\alpha \rightarrow 1$, i.e. near turning point, let $x = A - \xi$, we have

$$\left| \frac{k'}{k^2} \right| \sim \frac{l^2 A}{(2A\xi)^{\frac{3}{2}}} = \frac{l^2}{2^{\frac{3}{2}}\sqrt{A}\xi^{\frac{3}{2}}} \quad (12)$$

at the edge of the validity region,

$$\left| \frac{k'}{k^2} \right| \sim 1 \Rightarrow \xi \sim 2^{\frac{7}{6}}l \left(n + \frac{1}{2} \right)^{-\frac{1}{6}}. \quad (13)$$

Thus the fraction of the classically allowed region occupied by this boundary layer is

$$\frac{\xi}{A} \sim \frac{1}{2^{5/3}} \left(n + \frac{1}{2} \right)^{-2/3}, \quad (14)$$

which scales with decreasing n . Thus, although the WKB criterion always fails arbitrarily close to the turning points, the “bad” region becomes a parametrically small fraction of the classically allowed interval as n increases.

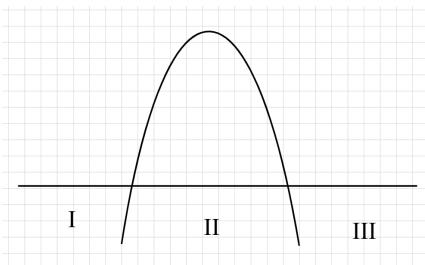
Consider the general scattering problem from a potential barrier with classical turning points at $x = a$ and $x = b$ (where $b > a$). Assuming that the WKB approximation holds, the wavefunction in each region can be written as

$$\begin{aligned}\psi_{x < a} &= \frac{A}{\sqrt{k(x)}} e^{i \int_a^x k(x') dx'} + \frac{B}{\sqrt{k(x)}} e^{-i \int_a^x k(x') dx'} \\ \psi_{a < x < b} &= \frac{C}{\sqrt{\kappa(x)}} e^{-\int_a^x \kappa(x') dx'} + \frac{D}{\sqrt{\kappa(x)}} e^{\int_a^x \kappa(x') dx'} \\ \psi_{x > b} &= \frac{F}{\sqrt{k(x)}} e^{i \int_b^x k(x') dx'} + \frac{G}{\sqrt{k(x)}} e^{-i \int_b^x k(x') dx'},\end{aligned}$$

with $k(x) = \sqrt{2m(E - V(x))}/\hbar$ and $\kappa(x) = \sqrt{2m(V(x) - E)}/\hbar$. Use the WKB method to compute the 2×2 matrix \mathcal{M} , defined by

$$\begin{pmatrix} A \\ B \end{pmatrix} = \mathcal{M} \begin{pmatrix} F \\ G \end{pmatrix},$$

in terms of the parameter $\theta = \exp \left[\int_a^b \kappa(x') dx' \right]$. For $G = 0$ (no incoming wave from the right), write down the transmission coefficient \tilde{T} in the limit of a high and broad barrier ($\theta \gg 1$).



First, label $\psi_{x < a} = \psi_I$, $\psi_{a < x < b} = \psi_{II}$, $\psi_{x > b} = \psi_{III}$. We will reformulate the wavefunctions in each region and connect them using connection formulas at the turning points $x = a, b$. We plot the potential with the regions marked below (See left).

Let's follow the order $\psi_{III} \rightarrow \psi_{II} \rightarrow \psi_I$.

- First, write ψ_{III} as follows:

$$\begin{aligned}\frac{F}{\sqrt{k(x)}} \exp \left(i \int_b^x k(x') dx' \right) &= \frac{F}{\sqrt{k}} e^{i \frac{\pi}{4}} e^{i \varphi}, \\ \frac{G}{\sqrt{k(x)}} \exp \left[i \int_b^x k(x') dx' \right] &\equiv \frac{G}{\sqrt{k}} e^{-i \frac{\pi}{4}} e^{-i \varphi}\end{aligned}\tag{15}$$

where $\varphi \equiv \int_k^x k(x') dx - i\pi/4$. Then we use Euler's formula to convert to

$$\begin{aligned}\psi_{III} &= \frac{1}{\sqrt{k}} [F e^{i \frac{\pi}{4}} (\cos \varphi + i \sin \varphi) + G e^{-i \frac{\pi}{4}} (\cos \varphi - i \sin \varphi)] \\ &= \frac{2}{\sqrt{k}} \cos \varphi \frac{1}{2} (F e^{i \frac{\pi}{4}} + G e^{-i \frac{\pi}{4}}) + \frac{1}{\sqrt{k}} \sin \varphi (i F e^{i \frac{\pi}{4}} - i G e^{-i \frac{\pi}{4}})\end{aligned}\tag{16}$$

and so each term can be connected to ψ_{II} using the connection formulas:

$$\psi_{II} = \frac{1}{\sqrt{\kappa}} \frac{1}{2} [F e^{i \frac{\pi}{4}} + G e^{-i \frac{\pi}{4}}] \exp \left(\int_b^x \kappa(x') dx' \right) - \frac{1}{\sqrt{\kappa}} (i F e^{i \frac{\pi}{4}} - i G e^{-i \frac{\pi}{4}}) \exp \left[- \int_b^x \kappa(x') dx' \right].\tag{17}$$

Using $\theta \equiv \exp \left[\int_a^b \kappa(x') dx' \right]$, we match the region of integration to get

$$\begin{aligned}
\psi_{II} &= \frac{1}{\sqrt{\kappa}} \frac{1}{2} [F e^{i\frac{\pi}{4}} + G e^{-i\frac{\pi}{4}}] \exp \left(\int_b^x \kappa(x') dx' + \int_a^b \kappa(x') dx' - \int_a^b \kappa(x') dx' \right) \\
&\quad - \frac{1}{\sqrt{\kappa}} (i F e^{i\frac{\pi}{4}} - i G e^{-i\frac{\pi}{4}}) \exp \left[- \int_b^x \kappa(x') dx' - \int_a^b \kappa(x') dx' + \int_a^b \kappa(x') dx' \right] \\
&= \frac{1}{\sqrt{\kappa}} \frac{1}{2} [F e^{i\frac{\pi}{4}} + G e^{-i\frac{\pi}{4}}] \frac{1}{\theta} \exp \left(\int_a^x \kappa(x') dx' \right) - \frac{1}{\sqrt{\kappa}} (i F e^{i\frac{\pi}{4}} - i G e^{-i\frac{\pi}{4}}) \theta \exp \left[- \int_a^x \kappa(x') dx' \right].
\end{aligned} \tag{18}$$

From which we read off

$$C = \theta [i G e^{-i\frac{\pi}{4}} - i F e^{i\frac{\pi}{4}}], \quad D = \frac{1}{2\theta} [F e^{i\frac{\pi}{4}} + G e^{-i\frac{\pi}{4}}]. \tag{19}$$

- Now we connect ψ_{II} to ψ_I using the same procedure. We first note ψ_{II} :

$$\psi_{II} = \frac{C}{\sqrt{\kappa(x)}} \exp \left[- \int_a^x \kappa(x') dx' \right] + \frac{D}{\sqrt{\kappa(x)}} \exp \left[\int_a^x \kappa(x') dx' \right]. \tag{20}$$

At the turning point $x = a$, the potential has positive slope $V'(a) > 0$. Applying connection formulas term-by-term to ψ_{II} gives

$$\psi_I = \frac{2C}{\sqrt{k(x)}} \cos \left[\int_x^a k - \frac{\pi}{4} \right] - \frac{D}{\sqrt{k(x)}} \sin \left[\int_x^a k - \frac{\pi}{4} \right]. \tag{21}$$

Let $\varphi_a \equiv \int_a^x k(x') dx'$, so $\int_x^a k = -\varphi_a$. Then

$$\cos \left[\int_x^a k - \frac{\pi}{4} \right] = \cos \left[-\varphi_a - \frac{\pi}{4} \right] = \cos \left(\varphi_a + \frac{\pi}{4} \right), \tag{22}$$

$$\sin \left[\int_x^a k - \frac{\pi}{4} \right] = \sin \left[-\varphi_a - \frac{\pi}{4} \right] = -\sin \left(\varphi_a + \frac{\pi}{4} \right). \tag{23}$$

Thus

$$\psi_I = \frac{2C}{\sqrt{k}} \cos \left(\varphi_a + \frac{\pi}{4} \right) - \frac{D}{\sqrt{k}} \left[-\sin \left(\varphi_a + \frac{\pi}{4} \right) \right] = \frac{1}{\sqrt{k}} \left[2C \cos \left(\varphi_a + \frac{\pi}{4} \right) + D \sin \left(\varphi_a + \frac{\pi}{4} \right) \right]. \tag{24}$$

Let $\tilde{\varphi} \equiv \varphi_a + \frac{\pi}{4}$. Using Euler's formula,

$$\psi_I = \frac{1}{\sqrt{k}} \left[2C \frac{e^{i\tilde{\varphi}} + e^{-i\tilde{\varphi}}}{2} + D \frac{e^{i\tilde{\varphi}} - e^{-i\tilde{\varphi}}}{2i} \right] \tag{25}$$

$$= \frac{1}{\sqrt{k}} \left[C(e^{i\tilde{\varphi}} + e^{-i\tilde{\varphi}}) + \left(\frac{D}{2i} \right) (e^{i\tilde{\varphi}} - e^{-i\tilde{\varphi}}) \right] \tag{26}$$

$$= \frac{1}{\sqrt{k}} \left[e^{i\tilde{\varphi}} \left(C + \frac{D}{2i} \right) + e^{-i\tilde{\varphi}} \left(C - \frac{D}{2i} \right) \right]. \tag{27}$$

Since $\frac{D}{2i} = -i\frac{D}{2}$, this is

$$\psi_I = \frac{1}{\sqrt{k}} \left[e^{i\tilde{\varphi}} \left(C - i\frac{D}{2} \right) + e^{-i\tilde{\varphi}} \left(C + i\frac{D}{2} \right) \right]. \tag{28}$$

Substituting $\tilde{\varphi} = \varphi_a + \frac{\pi}{4}$,

$$\begin{aligned}\psi_I &= \frac{1}{\sqrt{k}} \left[e^{i(\varphi_a + \frac{\pi}{4})} \left(C - i \frac{D}{2} \right) + e^{-i(\varphi_a + \frac{\pi}{4})} \left(C + i \frac{D}{2} \right) \right] \\ &= \frac{1}{\sqrt{k}} \left[e^{i\frac{\pi}{4}} \left(C - i \frac{D}{2} \right) e^{i\varphi_a} + e^{-i\frac{\pi}{4}} \left(C + i \frac{D}{2} \right) e^{-i\varphi_a} \right].\end{aligned}\tag{29}$$

Comparing to $\psi_I = \frac{A}{\sqrt{k}} e^{i\varphi_a} + \frac{B}{\sqrt{k}} e^{-i\varphi_a}$, we read off

$$A = e^{i\frac{\pi}{4}} \left(C - i \frac{D}{2} \right), \quad B = e^{-i\frac{\pi}{4}} \left(C + i \frac{D}{2} \right).\tag{30}$$

Now substitute the expressions for C and D :

$$C = \theta [iGe^{-i\frac{\pi}{4}} - iFe^{i\frac{\pi}{4}}], \quad D = \frac{1}{2\theta} [Fe^{i\frac{\pi}{4}} + Ge^{-i\frac{\pi}{4}}].\tag{31}$$

For A ,

$$\begin{aligned}A &= e^{i\frac{\pi}{4}} \left[\theta(iGe^{-i\frac{\pi}{4}} - iFe^{i\frac{\pi}{4}}) - \frac{i}{2} \frac{1}{2\theta} (Fe^{i\frac{\pi}{4}} + Ge^{-i\frac{\pi}{4}}) \right] \\ &= e^{i\frac{\pi}{4}} \left[i\theta(Ge^{-i\frac{\pi}{4}} - Fe^{i\frac{\pi}{4}}) - \left(\frac{i}{4\theta} \right) (Fe^{i\frac{\pi}{4}} + Ge^{-i\frac{\pi}{4}}) \right] \\ &= \left(\theta + \frac{1}{4\theta} \right) F + i \left(\theta - \frac{1}{4\theta} \right) G.\end{aligned}\tag{32}$$

For B ,

$$\begin{aligned}B &= e^{-i\frac{\pi}{4}} \left[\theta(iGe^{-i\frac{\pi}{4}} - iFe^{i\frac{\pi}{4}}) + \frac{i}{2} \frac{1}{2\theta} (Fe^{i\frac{\pi}{4}} + Ge^{-i\frac{\pi}{4}}) \right] \\ &= e^{-i\frac{\pi}{4}} \left[i\theta(Ge^{-i\frac{\pi}{4}} - Fe^{i\frac{\pi}{4}}) + \left(\frac{i}{4\theta} \right) (Fe^{i\frac{\pi}{4}} + Ge^{-i\frac{\pi}{4}}) \right] \\ &= i \left(\frac{1}{4\theta} - \theta \right) F + \left(\theta + \frac{1}{4\theta} \right) G.\end{aligned}\tag{33}$$

This gives the transfer matrix relation

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \theta + \frac{1}{4\theta} & i(\theta - \frac{1}{4\theta}) \\ i(\frac{1}{4\theta} - \theta) & \theta + \frac{1}{4\theta} \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix}.\tag{34}$$

In the limit $G = 0$, and $\theta \gg 1$, we have

$$A = \left(\theta + \frac{1}{4\theta} \right) F, \quad B = i \left(\frac{1}{4\theta} - \theta \right) F\tag{35}$$

Transmission is given by

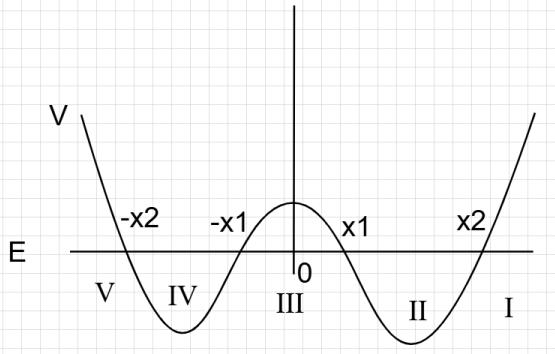
$$T = \left| \frac{F}{A} \right|^2 = \frac{1}{(\theta + \frac{1}{4\theta})^2} \sim \frac{1}{\theta^2} = \exp \left[-2 \int_a^b \kappa(x') dx' \right]\tag{36}$$

3

A particle of mass m and energy E is in a one-dimensional symmetric double well potential $V(x)$ centered at $x = 0$, where $V(x) \rightarrow \infty$ for $x \rightarrow \pm\infty$ and $V_0 = V(x = 0)$ is the maximum height of the central barrier.

Taking $E < V_0$, use the WKB method to determine the energy quantization conditions in terms of the quantities $\theta = \int_{x_1}^{x_2} k(x') dx'$ and $\phi = \int_{-x_1}^{x_1} \kappa(x') dx'$, where the classical turning points are $x = \pm x_1$ and $x = \pm x_2$, with $x_2 > x_1$. Describe the behavior in the limit of a high and broad barrier (large ϕ).

(Hint: exploit the parity of this potential.)



See left for the 1D symmetric double well potential, with marked regions and turning points. We will exploit the symmetry and parity of the potential in our derivation, in that we only solve for the region $x > 0$.

We propose the following wavefunction ansatz for each region (symmetry about $x = 0$ allows us to only consider $x > 0$):

$$\begin{aligned}\psi_I &= \frac{F}{\sqrt{\kappa}} e^{-\int_{x_2}^x \kappa dx'} \\ \psi_{\text{II}} &= \frac{1}{\sqrt{k}} \left[A \cos\left(s - \frac{\pi}{4}\right) + B \sin\left(s - \frac{\pi}{4}\right) \right], \quad \left(s \equiv \int_{x_1}^x k(x') dx' \right) \\ \psi_{\text{III}} &= \frac{1}{\sqrt{\kappa}} [C e^{u(x)} + D e^{-u(x)}], \quad \left(u(x) \equiv \int_0^x \kappa(x') dx' \right)\end{aligned}\tag{37}$$

We connect ψ_I to ψ_{II} at turning point $x = x_2$ where $V'(x_2) > 0$. Using connection formulas, we convert $\psi_I \rightarrow \psi_{\text{II}}$ as

$$\begin{aligned}\psi_{\text{II}} &\propto \frac{2}{\sqrt{k}} \cos\left(\int_x^{x_2} k(x') dx' - \frac{\pi}{4}\right) = \frac{2}{\sqrt{k}} \cos\left(\theta - \int_{x_1}^x k dx' - \frac{\pi}{4}\right) \\ &= \frac{2}{\sqrt{k}} \left[\cos \theta \cos\left(\int_{x_1}^x k dx' + \frac{\pi}{4}\right) + \sin \theta \sin\left(\int_{x_1}^x k dx' + \frac{\pi}{4}\right) \right] \\ &= \frac{2}{\sqrt{k}} \left[\sin \theta \cos\left(s - \frac{\pi}{4}\right) - \cos \theta \sin\left(s - \frac{\pi}{4}\right) \right]\end{aligned}\tag{38}$$

Matching coefficients with original ψ_{II} , we read off

$$\begin{aligned}A &= 2 \sin \theta, \quad B = -2 \cos \theta \\ \Rightarrow \frac{B}{A} &= -\cot \theta\end{aligned}\tag{39}$$

We next connect ψ_{II} to ψ_{III} at turning point $x = x_1$ where $V'(x_1) < 0$. Using connection formulas, we convert $\psi_{\text{II}} \rightarrow \psi_{\text{III}}$ by first writing

$$\psi_{\text{II}} = \frac{A}{2} \frac{2}{\sqrt{k}} \cos\left(s - \frac{\pi}{4}\right) + \frac{B}{\sqrt{k}} \sin\left(s - \frac{\pi}{4}\right)\tag{40}$$

then

$$\psi_{\text{III}} \propto \frac{1}{\sqrt{\kappa}} \left[\frac{A}{2} \exp \left(\int_{x_1}^x \kappa dx' \right) - B \exp \left(- \int_{x_1}^x \kappa dx' \right) \right] \quad (41)$$

since $\int_{x_1}^x \kappa dx' = \int_0^x \kappa dx' - \int_0^{x_1} \kappa dx' = u - \frac{\varphi}{2}$, we can write

$$\psi_{\text{III}} \propto \frac{1}{\sqrt{\kappa}} \left[\frac{A}{2} \exp \left(u - \frac{\varphi}{2} \right) - B \exp \left(- \left(u - \frac{\varphi}{2} \right) \right) \right] = \frac{1}{\sqrt{\kappa}} \left[\left(\frac{A}{2} e^{-\frac{\varphi}{2}} \right) e^u - \left(B e^{\frac{\varphi}{2}} \right) e^{-u} \right] \quad (42)$$

Matching coefficients with original ψ_{III} , we read off

$$C = \frac{A}{2} e^{-\frac{\varphi}{2}}, \quad D = -B e^{\frac{\varphi}{2}} \quad (43)$$

Symmetry of the potential $V(-x) = V(x)$ means all eigenstates are either even ($\psi(-x) = \psi(x)$) or odd ($\psi(-x) = -\psi(x)$). Since we're only working on $x > 0$, we impose the parity condition at the center $x = 0$ (where $u(0) = 0$) to fix the coefficients C, D in ψ_{III} . This automatically determines the solution for $x < 0$ by reflection.

- **Even states** ($\psi'(0) = 0$): The wavefunction in the barrier is

$$\psi_{\text{III}(x)} \propto \frac{1}{\sqrt{\kappa(x)}} [C e^{u(x)} + D e^{-u(x)}]. \quad (44)$$

Differentiate:

$$\psi'_{\text{III}}(x) \propto \frac{1}{\sqrt{\kappa(x)}} [C \kappa(x) e^{u(x)} - D \kappa(x) e^{-u(x)}] \quad (45)$$

(the $\kappa(x)$ factor comes from the chain rule on the exponentials, and the $\frac{1}{\sqrt{\kappa}}$ prefactor derivative is neglected in WKB as it's slowly varying). Set $\psi'_{\text{III}}(0) = 0$: at $x = 0, u = 0$, so $e^u = e^{-u} = 1$, giving

$$C \kappa(0) - D \kappa(0) = 0 \Rightarrow C = D \quad (46)$$

Now plug in the expressions for C, D from the connection at x_1 :

$$C = \frac{A}{2} e^{-\frac{\varphi}{2}}, \quad D = -B e^{+\frac{\varphi}{2}} \quad (47)$$

So

$$\frac{A}{2} e^{-\frac{\varphi}{2}} = -B e^{+\frac{\varphi}{2}} \Rightarrow \frac{B}{A} = -\frac{1}{2} e^{-\varphi} \quad (48)$$

But from the connection at x_2 , we have $\frac{B}{A} = -\cot \theta$. Thus:

$$\cot \theta = +\frac{1}{2} e^{-\varphi}, \quad (49)$$

which is the quantization condition for even states.

- **Odd states** ($\psi(0) = 0$): Evaluate $\psi_{\text{III}(0)}$: at $x = 0, u = 0$, so $e^u = e^{-u} = 1$, giving

$$C + D = 0 \Rightarrow C = -D \quad (50)$$

Plug in C, D :

$$\frac{A}{2} e^{-\frac{\varphi}{2}} = -(-B e^{+\frac{\varphi}{2}}) \Rightarrow \frac{B}{A} = +\frac{1}{2} e^{-\varphi}. \quad (51)$$

Again using $\frac{B}{A} = -\cot \theta$ from x_2 :

$$\cot \theta = -\frac{1}{2} e^{-\varphi}, \quad (52)$$

which is the quantization condition for odd states.

Collectively, the quantization conditions for even and odd states are:

$$\begin{aligned} \text{Odd : } \cot \theta &= -\frac{1}{2}e^{-\varphi} \\ \text{Even : } \cot \theta &= +\frac{1}{2}e^{-\varphi} \end{aligned} \quad (53)$$

with

$$\theta = \int_{x_1}^{x_2} k(x') dx', \quad \varphi = 2 \int_0^{x_1} \kappa(x') dx'. \quad (54)$$

Notedly, as $\varphi \rightarrow \infty$ both conditions reduces to

$$\cot \theta = 0 \Rightarrow \theta(E) = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots = \left(n + \frac{1}{2}\right)\pi \quad (55)$$

which is exactly the quantization condition for a single isolated well, as expected since large φ means a high/wide barrier that decouples the wells.

4

(a) Compute $K(x, t; x', 0)$ for a particle of mass m subject to a constant force F in one dimension, using the knowledge that this quantity can be written as $A(t)e^{iS_{\text{classical}}/\hbar}$, where $S_{\text{classical}}$ is the action evaluated along the classical path.

(b) Repeat (a) but for the simple harmonic oscillator in one dimension with mass m and frequency ω . [For the case of the harmonic oscillator, you do not need to evaluate $A(t)$ explicitly.]

a.

For a particle moving under F from $x = x', t = 0$, we have its EOM:

$$x_{\text{CL}}(t) = x' + v_0 t + \frac{1}{2} a t^2 = x' + \left(\frac{x - x'}{t} - \frac{Ft}{2m} \right) t' + \frac{F}{2m} t^2 \quad (56)$$

and so the classical action is given as

$$S = \int_0^t L dt = \int_0^t \frac{1}{2} m \dot{x}^2 + Fx(t') dt' = \frac{m(x - x')^2}{2t} + \frac{F(x + x')t}{2} - \frac{F^2 t^3}{24m}. \quad (57)$$

The propagator K is thus

$$K = A(t) \exp(iS/\hbar) \quad (58)$$

where $A(t)$ can be evaluated by considering the free particle limit $F \rightarrow 0$:

$$K = \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left(\frac{i m(x - x')^2}{2\hbar t}\right) \equiv A(t) \exp\left(\frac{i m(x - x')^2}{2\hbar t}\right) \Rightarrow A(t) = \sqrt{\frac{m}{2\pi i \hbar t}}. \quad (59)$$

Therefore, the full propagator is

$$K = \sqrt{\frac{m}{2\pi i \hbar t}} \exp\left[\frac{i m(x - x')^2}{2t} + \frac{F(x + x')t}{2} - \frac{F^2 t^3}{24m}\right]. \quad (60)$$

b.

For the simple harmonic oscillator, the classical Lagrangian is given as

$$L = T - V = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2 \quad (61)$$

and the EOM is retrieved as

$$\frac{d}{dt}(m\dot{x}) + m\omega^2 x = 0 \Rightarrow \ddot{x}\omega^2 x = 0 \quad (62)$$

the solution to the EOM with boundary conditions $x(0) = x', x(t) = x$ is

$$x_{cl}(\tau) = \frac{x' \sin(\omega(t - \tau)) + x \sin(\omega\tau)}{\sin(\omega t)} \quad (63)$$

the classical action is evaluated as

$$S = \int_0^t L d\tau = \int_0^t \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2 d\tau = \int_0^t \frac{m}{2} \frac{d}{d\tau}(x\dot{x}) d\tau = \frac{m}{2} [x(t)\dot{x}(t) - x(0)\dot{x}(0)] \quad (64)$$

where

$$\begin{aligned} \dot{x}(\tau) &= \frac{\omega}{\sin \omega t} (-x' \cos(\omega(t - \tau)) + x \cos(\omega\tau)) \\ \Rightarrow \dot{x}(0) &= \frac{\omega}{\sin \omega t} (-x' \cos \omega t + x), \quad \dot{x}(t) = \frac{\omega}{\sin \omega t} (-x' + x \cos \omega t) \end{aligned} \quad (65)$$

Plugging in, we have

$$S = \frac{m\omega}{2 \sin \omega t} [(x^2 + x'^2) \cos \omega t - 2xx'] \quad (66)$$

The propagator is thus

$$K = A(t) \exp\left(\frac{i}{\hbar} \frac{m\omega}{2 \sin \omega t} [(x^2 + x'^2) \cos \omega t - 2xx']\right) \quad (67)$$

For the simple harmonic oscillator in one dimension with mass m and frequency ω , recalling that

$$K(x, t; x', 0) = \sum_n \psi_n(x) \psi_n^*(x') e^{-iE_n t/\hbar},$$

use this expression (taking $x = x' = 0$) to determine the energy eigenvalues E_n up through $n = 4$. Can all of the eigenvalues through $n = 4$ be obtained in this way?

For $x = x' = 0$, we have

$$K = \sum_n |\psi_n(0)|^2 e^{-iE_n t/\hbar}, \quad (68)$$

while for the harmonic oscillator, we recall its propagator in closed form (with $x = x' = 0$)

$$K = \left(\frac{m\omega}{2\pi i \hbar \sin \omega t} \right)^{1/2} = \left(\frac{m\omega}{\pi \hbar e^{i\omega t} (1 - e^{-2i\omega t})} \right)^{-1/2} = \sqrt{\frac{m\omega}{\pi \hbar}} e^{-i\omega t/2} (1 - e^{-2i\omega t})^{1/2} \quad (69)$$

Using binomial expansion, i.e.

$$(1 - z)^{-1/2} = \sum_{k=0}^{\infty} \frac{(2k)!}{4^k (k!)^2} z^k \quad (70)$$

taking $z = e^{-2i\omega t}$, we have

$$K = \sqrt{m\omega \pi \hbar} e^{-i\omega t/2} \sum_{k=0}^{\infty} \frac{(2k)!}{4^k (k!)^2} (e^{-2i\omega t})^k = \sqrt{\frac{m\omega}{\pi \hbar}} \sum_{k=0}^{\infty} \frac{(2k)!}{4^k (k!)^2} e^{(-i\omega t)(2k+1/2)} \quad (71)$$

Also, recall that the Harmonic oscillator has wavefunction solutions in terms of Hermite polynomials:

$$\psi_n = N_n H(\alpha x) e^{-\alpha^2 x^2/2} \quad (72)$$

where $\alpha = \sqrt{m\omega/\hbar}$, and N_n is the normalization constant. Notedly, $H_n(0) = 0$ for odd n , so $\psi_n(0) = 0$ for odd n . We can thus rewrite Equation 68 in terms of only even $n = 2k$:

$$K = \sum_{k=0}^{\infty} |\psi_{2k}(0)|^2 e^{-iE_{2k} t/\hbar} \quad (73)$$

Matching with Equation 71, we identify

$$\sum_k |\psi_{2k}(0)|^2 e^{-iE_{2k} t/\hbar} = \sqrt{\frac{m\omega}{\pi \hbar}} \sum_{k=0}^{\infty} \frac{(2k)!}{4^k (k!)^2} e^{-i\omega t(2k+1/2)} \quad (74)$$

and so the time dependent terms must match for each k :

$$E_{2k} t / \hbar = \left(2k + \frac{1}{2} \right) \omega t \Rightarrow E_n = \hbar \omega \left(n + \frac{1}{2} \right) \quad (75)$$

We can therefore determine energy eigenvalues for even n :

$$E_0 = \frac{1}{2} \hbar \omega; \quad E_2 = \frac{5}{2} \hbar \omega; \quad E_4 = \frac{9}{2} \hbar \omega; \dots \quad (76)$$

However, not all of the eigenvalues through $n = 4$ can be obtained using this method. As mentioned, the wavefunctions for odd quantum numbers ($n = 1, 3, 5, \dots$) have odd parity and are therefore zero at the origin, $\psi_n(0) = 0$. These states make no contribution to the spectral sum for $K(0, t; 0, 0)$ and are thus “invisible” to this specific analysis.