AQM 831 — ADVANCED QUANTUM MECHANICS-1

Name: AKIFUL ISLAM ZAWAD **Date:** December 29, 2024

Track Follower: 2 **Assessment:** Final Examination (Zeta)

1. Consider the time-independent Hamilton-Jacobi equation:

$$H\left(q, \frac{\partial S}{\partial q}\right) = E \tag{1}$$

for a charged particle in an electric field with potential:

$$V(r) = \frac{e}{r}. \tag{2}$$

(a) Substituting $S = k \ln \psi$, derive

$$\sum_{q_i=x,y,z} \left(\frac{\partial \psi}{\partial q_i}\right)^2 - \frac{2m}{k^2}\left(E + \frac{e^2}{r}\right)\psi^2 = 0. \tag{3}$$

(b) Define the action:

$$J = \int\int\int dx\,dy\,dz \left[\left(\frac{\partial \psi}{\partial x}\right)^2 + \left(\frac{\partial \psi}{\partial y}\right)^2 + \left(\frac{\partial \psi}{\partial z}\right)^2 - \frac{2m}{k^2}\left(E + \frac{e^2}{r}\right)\psi^2\right]. \tag{4}$$

Find a $\psi(x, y, z)$ which is stationary for an arbitrary variation of J over the whole coordinate space.

(c) Discuss the significance of the coefficient k.

Solution 1(a)

The time-independent Hamilton-Jacobi equation is:

$$H\left(q, \frac{\partial S}{\partial q}\right) = E, \tag{5}$$

where $H(q, p)$ is the Hamiltonian. For a charged particle in an electric potential:

$$H = \frac{p^2}{2m} + V(r) = \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + V(r). \tag{6}$$

Substituting $S = k \ln \psi$:

$$\frac{\partial S}{\partial q_i} = \frac{\partial}{\partial q_i}(k \ln \psi) = k\frac{1}{\psi}\frac{\partial \psi}{\partial q_i}$$
$$\left(\frac{\partial S}{\partial q}\right)^2 = \sum_{q_i=x,y,z}\left(\frac{\partial S}{\partial q_i}\right)^2$$

$$
\begin{aligned}
&= \sum_{q_i=x,y,z} \left(k \frac{1}{\psi} \frac{\partial \psi}{\partial q_i} \right)^2 \\
&= k^2 \sum_{q_i=x,y,z} \left(\frac{1}{\psi} \frac{\partial \psi}{\partial q_i} \right)^2 \\
&= \frac{k^2}{\psi^2} \sum_{q_i=x,y,z} \left(\frac{\partial \psi}{\partial q_i} \right)^2 .
\end{aligned} \tag{7}
$$

Substitute into (6):

$$
\frac{1}{2m} \frac{k^2}{\psi^2} \sum_{q_i=x,y,z} \left(\frac{\partial \psi}{\partial q_i} \right)^2 + \frac{e^2}{r} = E. \tag{8}
$$

Multiply through by $2m\psi^2/k^2$:

$$
\sum_{q_i=x,y,z} \left(\frac{\partial \psi}{\partial q_i} \right)^2 - \frac{2m}{k^2} \left(E + \frac{e^2}{r} \right) \psi^2 = 0 \tag{9}
$$

$$
\sum_{q_i=x,y,z} \left(\frac{\partial \psi}{\partial q_i} \right)^2 - \frac{2m}{k^2} \left(E + \frac{e^2}{r} \right) \psi^2 = 0. \tag{10}
$$

Solution 1(b)

The action J is defined as:

$$
J = \int \int \int dx\, dy\, dz \Bigg[\left(\frac{\partial \psi}{\partial x} \right)^2 + \left(\frac{\partial \psi}{\partial y} \right)^2 + \left(\frac{\partial \psi}{\partial z} \right)^2 - \frac{2m}{k^2} \left(E + \frac{e^2}{r} \right) \psi^2 \Bigg]. \tag{11}
$$

To find $\psi(x, y, z)$ that makes J stationary, consider an arbitrary variation of ψ:

$$
\psi \to \psi + \delta\psi. \tag{12}
$$

The variation in J (11) is:

$$
\delta J = \int \int \int dx\, dy\, dz \Bigg[2 \frac{\partial \psi}{\partial x} \frac{\partial (\delta\psi)}{\partial x} + 2 \frac{\partial \psi}{\partial y} \frac{\partial (\delta\psi)}{\partial y} + 2 \frac{\partial \psi}{\partial z} \frac{\partial (\delta\psi)}{\partial z} - \frac{4m}{k^2} \left(E + \frac{e^2}{r} \right) \psi \delta\psi \Bigg]. \tag{13}
$$

Consider the first term:

$$
\int \int \int dx\, dy\, dz\, 2 \frac{\partial \psi}{\partial x} \frac{\partial (\delta\psi)}{\partial x}.
$$

Use the product rule for differentiation:

$$
\frac{\partial}{\partial x} \left(\frac{\partial \psi}{\partial x} \delta\psi \right) = \frac{\partial^2 \psi}{\partial x^2} \delta\psi + \frac{\partial \psi}{\partial x} \frac{\partial (\delta\psi)}{\partial x}
$$

$$\therefore \frac{\partial\psi}{\partial x}\frac{\partial(\delta\psi)}{\partial x} = \frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\delta\psi\right) - \frac{\partial^2\psi}{\partial x^2}\delta\psi. \tag{14}$$

Substitute into the integral:

$$\begin{aligned}\int\int\int dx\,dy\,dz\,2\frac{\partial\psi}{\partial x}\frac{\partial(\delta\psi)}{\partial x} &= \int\int\int dx\,dy\,dz\,2\left[\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\delta\psi\right) - \frac{\partial^2\psi}{\partial x^2}\delta\psi\right]\\ &= 2\int\int\int dx\,dy\,dz\,\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\delta\psi\right) - 2\int\int\int dx\,dy\,dz\,\frac{\partial^2\psi}{\partial x^2}\delta\psi.\end{aligned}$$

For the first term, the divergence theorem ensures this boundary term vanishes because ψ and $\delta\psi$ are zero at infinity:

$$\int\int\int dx\,dy\,dz\,\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\delta\psi\right) = 0. \tag{15}$$

Thus:

$$\int\int\int dx\,dy\,dz\,2\frac{\partial\psi}{\partial x}\frac{\partial(\delta\psi)}{\partial x} = -2\int\int\int dx\,dy\,dz\,\frac{\partial^2\psi}{\partial x^2}\delta\psi.$$

Repeat the same process for the y- and z-components:

$$\begin{aligned}\int\int\int dx\,dy\,dz\,2\frac{\partial\psi}{\partial y}\frac{\partial(\delta\psi)}{\partial y} &= -2\int\int\int dx\,dy\,dz\,\frac{\partial^2\psi}{\partial y^2}\delta\psi,\\ \int\int\int dx\,dy\,dz\,2\frac{\partial\psi}{\partial z}\frac{\partial(\delta\psi)}{\partial z} &= -2\int\int\int dx\,dy\,dz\,\frac{\partial^2\psi}{\partial z^2}\delta\psi.\end{aligned}$$

Substitute back into δJ:

$$\begin{aligned}\delta J &= \int\int\int dx\,dy\,dz\left[-2\frac{\partial^2\psi}{\partial x^2}\delta\psi - 2\frac{\partial^2\psi}{\partial y^2}\delta\psi - 2\frac{\partial^2\psi}{\partial z^2}\delta\psi - \frac{4m}{k^2}\left(E + \frac{e^2}{r}\right)\psi\delta\psi\right]\\ &= \int\int\int dx\,dy\,dz\,\delta\psi\left[-2\nabla^2\psi - \frac{4m}{k^2}\left(E + \frac{e^2}{r}\right)\psi\right]\\ &= \int\int\int dx\,dy\,dz\,\delta\psi\left[-2\nabla^2\psi - \frac{4m}{k^2}\left(E + \frac{e^2}{r}\right)\psi\right].\end{aligned} \tag{16}$$

For J to be stationary, $\delta J = 0$ for all $\delta\psi$. Thus:

$$\nabla^2\psi + \frac{2m}{k^2}\left(E + \frac{e^2}{r}\right)\psi = 0. \tag{17}$$

This is a form of the Schrödinger equation for the system, where $\psi(x, y, z)$ satisfies:

$$\psi(x, y, z) = \psi(r),$$

as the potential depends only on r.

Solution 1(c)

The coefficient k is a scaling parameter that connects the Hamilton-Jacobi formalism to the wavefunction formalism. Specifically:

- The value of k^2 is inversely proportional to $\hbar^2$, bridging the classical and quantum descriptions.
- The choice of k scales the amplitude of the wavefunction ψ and ensures consistency with the probabilistic interpretation of quantum mechanics.

---

2. Consider Laplace's equation:
   (a) Split Laplace's equation in spherical polar coordinates with and without azimuthal symmetry.
   (b) Derive the Legendre and Associate Legendre Differential Equations.
   (c) Using the Method of Frobenius, find the solution of the Legendre differential equation.
   (d) Find the expressions for Legendre and Associate Legendre Polynomials.
   (e) Derive their recurrence relations and evaluate their orthogonality and parity properties.

Solution 2(a)

The Laplace equation in spherical coordinates is:

$$\nabla^2\Phi = 0,$$

where the Laplacian in spherical coordinates is expressed as:

$$\nabla^2\Phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\phi^2}. \tag{18}$$

Assume the solution can be written as:

$$\Phi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi).$$

Substituting this into the Laplace equation:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial(R\Theta\Phi)}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial(R\Theta\Phi)}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2(R\Theta\Phi)}{\partial\phi^2} = 0. \tag{19}$$

Using separation of variables:

$$\frac{R'}{R} + \frac{\Theta'}{\Theta} + \frac{\Phi'}{\Phi} = 0,$$

we separate the radial, angular, and azimuthal parts.

Azimuthal symmetry: Assume azimuthal symmetry, meaning $\frac{\partial}{\partial \phi} = 0$. The Laplace equation (19) simplifies to:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \Phi}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \Phi}{\partial \theta}\right) = 0. \tag{20}$$

Assume a separable solution of the form:

$$\Phi(r,\theta) = R(r)\Theta(\theta). \tag{21}$$

Substitute $\Phi(r,\theta) = R(r)\Theta(\theta)$ into the equation:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial (R\Theta)}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial (R\Theta)}{\partial \theta}\right) = 0.$$

Since R and Θ are independent of each other:

$$\begin{aligned}
\frac{1}{r^2}\Theta\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{r^2 R}\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) &= 0. \\
\Theta\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + R\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) &= 0 \\
\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) &= 0.
\end{aligned} \tag{22}$$

Since the first term depends only on r and the second term depends only on θ, each term must equal a constant, which we denote as $-\ell(\ell+1)$. Thus:

$$\begin{aligned}
\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) &= \ell(\ell+1) \\
\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \ell(\ell+1)\Theta &= 0.
\end{aligned} \tag{23}$$

Without azimuthal symmetry: Separate the terms in (19):

$$\begin{aligned}
\frac{\Theta\Phi}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{R\Phi}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \frac{R\Theta}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\phi^2} &= 0 \\
\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{\Theta\Phi}\left(\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\Phi}{\partial\phi^2}\right) &= 0.
\end{aligned} \tag{24}$$

Since the first term depends only on r and the second term depends on θ and ϕ, separate variables by equating each part to a constant:

$$\begin{aligned}
\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) &= \ell(\ell+1) \\
\frac{1}{\Theta}\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2} &= -m^2.
\end{aligned} \tag{25}$$

The first equation describes the radial part, while the second describes the angular part.

The angular part of the separation gives:

$$
\begin{aligned}
\frac{1}{\Theta}\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\ell(\ell+1)-\frac{m^2}{\sin^2\theta}&=0\\
\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\ell(\ell+1)\sin\theta\Theta-\frac{m^2}{\sin\theta}\Theta&=0\\
\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left(\ell(\ell+1)\sin\theta-\frac{m^2}{\sin\theta}\right)\Theta&=0.
\end{aligned}
\tag{26}
$$

For $m=0$, the equation reduces to:

$$
\begin{aligned}
\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\ell(\ell+1)\sin\theta\Theta&=0\\
\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\ell(\ell+1)\Theta&=0.
\end{aligned}
$$

Substitute $x=\cos\theta$, so:

$$
\begin{aligned}
\sin\theta=\sqrt{1-x^2},\quad \frac{d}{d\theta}&=-\sqrt{1-x^2}\frac{d}{dx}\\
\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)&=\frac{d}{dx}\left[(1-x^2)\frac{d\Theta}{dx}\right].
\end{aligned}
$$

Substitute back:

$$
\frac{d}{dx}\left[(1-x^2)\frac{d\Theta}{dx}\right]+\ell(\ell+1)\Theta=0.
$$

Let $\Theta(x)=P_\ell(x)$, then:

$$
\begin{aligned}
\frac{d}{dx}\left[(1-x^2)\frac{dP_\ell}{dx}\right]+\ell(\ell+1)P_\ell&=0\\
(1-x^2)\frac{d^2P_\ell}{dx^2}-2x\frac{dP_\ell}{dx}+\ell(\ell+1)P_\ell&=0.
\end{aligned}
\tag{27}
$$

This is the Legendre differential equation.

Solution 2(b)

Assume a power series solution for $P_\ell(x)$:

$$
P_\ell(x)=\sum_{n=0}^{\infty}a_nx^n. \tag{28}
$$

The derivatives are:

$$
\frac{dP_\ell}{dx}=\sum_{n=1}^{\infty}na_nx^{n-1}, \tag{29}
$$

$$
\frac{d^2P_\ell}{dx^2}=\sum_{n=2}^{\infty}n(n-1)a_nx^{n-2}. \tag{30}
$$

Substitute these into the Legendre equation (27): Start with the first term:

$$(1-x^2)\frac{d^2P_\ell}{dx^2} = \left(1-x^2\right)\sum_{n=2}^{\infty} n(n-1)a_n x^{n-2}$$
$$(1-x^2)\frac{d^2P_\ell}{dx^2} = \sum_{n=2}^{\infty} n(n-1)a_n x^{n-2} - \sum_{n=2}^{\infty} n(n-1)a_n x^n$$

Rewrite the second sum by shifting $n \to n+2$:

$$\sum_{n=2}^{\infty} n(n-1)a_n x^{n-2} = \sum_{n=0}^{\infty} (n+2)(n+1)a_{n+2}x^n$$
$$(1-x^2)\frac{d^2P_\ell}{dx^2} = \sum_{n=0}^{\infty} (n+2)(n+1)a_{n+2}x^n - \sum_{n=2}^{\infty} n(n-1)a_n x^n. \tag{31}$$

For the second term:

$$-2x\frac{dP_\ell}{dx} = -2x\sum_{n=1}^{\infty} na_n x^{n-1}.$$

Shift $n \to n+1$:

$$-2x\frac{dP_\ell}{dx} = \sum_{n=0}^{\infty} -2(n+1)a_{n+1}x^n.$$

For the third term:

$$\ell(\ell+1)P_\ell = \ell(\ell+1)\sum_{n=0}^{\infty} a_n x^n.$$

Combine all terms:

$$\sum_{n=0}^{\infty}\Big[(n+2)(n+1)a_{n+2} - n(n-1)a_n - 2(n+1)a_{n+1} + \ell(\ell+1)a_n\Big]x^n = 0. \tag{32}$$

Since the series must vanish for all x, the coefficients must satisfy the following:

$$(n+2)(n+1)a_{n+2} - n(n-1)a_n - 2(n+1)a_{n+1} + \ell(\ell+1)a_n = 0. \tag{33}$$

Rearrange to find the recurrence relation:

$$a_{n+2} = \frac{(\ell+n+1)(\ell-n)}{(n+2)(n+1)}a_n. \tag{34}$$

The indicial equation comes from the lowest power of n, corresponding to $n=0$:

$$(\ell+1)\ell a_0 = 0. \tag{35}$$

Thus, ℓ is a non-negative integer for non-trivial solutions.

Solution 2(c)

The Legendre differential equation is:

$$(1-x^2)\frac{d^2P_\ell}{dx^2} - 2x\frac{dP_\ell}{dx} + \ell(\ell+1)P_\ell = 0. \tag{36}$$

Using the recurrence relation in (34) the series solution for $P_\ell(x)$ is:

$$P_\ell(x) = \sum_{n=0}^{\lfloor \ell/2 \rfloor} a_{2n}x^{\ell-2n}, \tag{37}$$

where the coefficients are determined recursively starting from $a_0 = 1$ (normalization can vary).

Explicitly:

$$a_{2n} = \frac{(-1)^n(2\ell-2n+1)(2\ell-2n+3)\cdots(\ell+1)}{(2n)!!}. \tag{38}$$

For specific values of ℓ, the Legendre polynomials are:

$$\begin{aligned}
P_0(x) &= 1, \\
P_1(x) &= x, \\
P_2(x) &= \frac{1}{2}(3x^2-1), \\
P_3(x) &= \frac{1}{2}(5x^3-3x), \\
P_4(x) &= \frac{1}{8}(35x^4-30x^2+3).
\end{aligned}$$

The Associated Legendre polynomials are solutions to:

$$(1-x^2)\frac{d^2P_\ell^m}{dx^2} - 2x\frac{dP_\ell^m}{dx} + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right]P_\ell^m = 0. \tag{39}$$

They are related to the Legendre polynomials $P_\ell(x)$ by:

$$P_\ell^m(x) = (1-x^2)^{|m|/2}\frac{d^{|m|}P_\ell}{dx^{|m|}}, \tag{40}$$

where $|m| \le \ell$.

For specific values of ℓ and m, the Associated Legendre polynomials are:

$$\begin{aligned}
&P_0^0(x) = 1, \\
&P_1^0(x) = x, \quad P_1^1(x) = -(1-x^2)^{1/2}, \\
&P_2^0(x) = \frac{1}{2}(3x^2-1), \quad P_2^1(x) = -3x(1-x^2)^{1/2}, \quad P_2^2(x) = 3(1-x^2), \\
&P_3^0(x) = \frac{1}{2}(5x^3-3x), \quad P_3^1(x) = -\frac{3}{2}(5x^2-1)(1-x^2)^{1/2}, \quad P_3^2(x) = 15x(1-x^2), \quad P_3^3(x) = -15(1-x^2)^{3/2}.
\end{aligned}$$

Solution 2(d)

These polynomials are orthogonal:

$$\int_{-1}^{1} P_\ell(x) P_{\ell'}(x)\, dx = \frac{2}{2\ell+1}\delta_{\ell\ell'} \tag{41}$$

$$\int_{-1}^{1} P_\ell^m(x) P_{\ell'}^m(x)\, dx = \frac{2(\ell+m)!}{(2\ell+1)(\ell-m)!}\delta_{\ell\ell'}. \tag{42}$$

The Legendre polynomials $P_\ell(x)$ satisfy the following recurrence relations:

1. First Recurrence Relation: From the Legendre equation:

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_\ell}{dx}\right] + \ell(\ell+1)P_\ell = 0. \tag{43}$$

Multiply through by x and rearrange:

$$x(2\ell+1)P_\ell = (\ell+1)P_{\ell+1} + \ell P_{\ell-1}. \tag{44}$$

Thus:

$$(\ell+1)P_{\ell+1}(x) = (2\ell+1)xP_\ell(x) - \ell P_{\ell-1}(x). \tag{45}$$

2. Derivative Relation: Differentiate the Legendre equation and simplify:

$$\frac{dP_\ell}{dx} = \ell P_{\ell-1}(x) - \ell x P_\ell(x). \tag{46}$$

3. Normalization of $P_\ell(1)$: Using the Rodrigues formula:

$$P_\ell(1) = 1, \quad P_\ell(-1) = (-1)^\ell. \tag{47}$$

Solution 2(e)

The Legendre polynomials are orthogonal over $[-1, 1]$:

$$\int_{-1}^{1} P_\ell(x) P_{\ell'}(x)\, dx = \frac{2}{2\ell+1}\delta_{\ell\ell'}. \tag{48}$$

Multiply the Legendre equation for $P_\ell(x)$ by $P_{\ell'}(x)$:

$$(1-x^2)\frac{d^2P_\ell}{dx^2}P_{\ell'} - 2x\frac{dP_\ell}{dx}P_{\ell'} + \ell(\ell+1)P_\ell P_{\ell'} = 0. \tag{49}$$

Multiply the equation for $P_{\ell'}(x)$ by $P_\ell(x)$:

$$(1-x^2)\frac{d^2P_{\ell'}}{dx^2}P_\ell - 2x\frac{dP_{\ell'}}{dx}P_\ell + \ell'(\ell'+1)P_{\ell'} P_\ell = 0. \tag{50}$$

Subtract these equations, integrate over $[-1,1]$, and use integration by parts to show that the orthogonality condition holds:

$$\int_{-1}^{1} P_\ell(x)P_{\ell'}(x)\,dx = 0 \quad \text{for} \quad \ell \neq \ell'. \tag{51}$$

Normalization: For $\ell = \ell'$, the integral evaluates to:

$$\int_{-1}^{1} P_\ell(x)^2\,dx = \frac{2}{2\ell+1}. \tag{52}$$

The parity of $P_\ell(x)$ is determined by the Rodrigues formula:

$$P_\ell(-x) = \frac{1}{2^\ell \ell!}\frac{d^\ell}{dx^\ell}[(x^2-1)^\ell]. \tag{53}$$

Substitute $-x$ for x and note that $(x^2-1)^\ell$ is even:

$$P_\ell(-x) = (-1)^\ell P_\ell(x). \tag{54}$$

Thus:

$$P_\ell(x) \text{ is even for even } \ell \text{ and odd for odd } \ell. \tag{55}$$

---

3. Answer the following questions:

   (a) Derive the associated Legendre recurrence relation:

$$P_\ell^{m+1}(x) + \frac{2mx}{\sqrt{1-x^2}}P_\ell^m(x) + \left[\ell(\ell+1) - m(m-1)\right]P_\ell^{m-1}(x) = 0. \tag{56}$$

   (b) Using the Rodriguez formula, show that $P_n(x)$ are orthogonal and:

$$\int_{-1}^{1} [P_n(x)]^2 dx = \frac{2}{2n+1}. \tag{57}$$

Solution 3(a)

The Legendre equation is:

$$(1-x^2)\frac{d^2P_\ell}{dx^2} - 2x\frac{dP_\ell}{dx} + \ell(\ell+1)P_\ell(x) = 0. \tag{58}$$

The associated Legendre function $P_\ell^m(x)$ is defined as:

$$P_\ell^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_\ell(x). \tag{59}$$

To differentiate $P_\ell^m(x)$, apply the product rule:

$$\frac{d}{dx}P_\ell^m(x) = \frac{d}{dx}\left[(1-x^2)^{m/2}\frac{d^m}{dx^m}P_\ell(x)\right]. \tag{60}$$

Using the product rule:

$$\frac{d}{dx}P_\ell^m(x) = \frac{d}{dx}\left[(1-x^2)^{m/2}\right]\frac{d^m}{dx^m}P_\ell(x) + (1-x^2)^{m/2}\frac{d}{dx}\left[\frac{d^m}{dx^m}P_\ell(x)\right]. \tag{61}$$

The derivative of $(1-x^2)^{m/2}$ is:

$$\frac{d}{dx}(1-x^2)^{m/2} = \frac{m}{2}(1-x^2)^{(m/2)-1}\cdot(-2x) = -mx(1-x^2)^{(m/2)-1}.$$

Substitute this into the expression for $\frac{d}{dx}P_\ell^m(x)$:

$$\frac{d}{dx}P_\ell^m(x) = -mx(1-x^2)^{(m/2)-1}\frac{d^m}{dx^m}P_\ell(x) + (1-x^2)^{m/2}\frac{d^{m+1}}{dx^{m+1}}P_\ell(x).$$

Next, apply the m-th derivative to the Legendre equation:

$$(1-x^2)\frac{d^2}{dx^2}\left[\frac{d^m}{dx^m}P_\ell(x)\right] - 2x\frac{d}{dx}\left[\frac{d^m}{dx^m}P_\ell(x)\right] + \ell(\ell+1)\frac{d^m}{dx^m}P_\ell(x) = 0.$$

First Term: Expand $(1-x^2)\frac{d^2}{dx^2}\left[\frac{d^m}{dx^m}P_\ell(x)\right]$ using the product rule:

$$(1-x^2)\frac{d^2}{dx^2}\left[\frac{d^m}{dx^m}P_\ell(x)\right] = (1-x^2)\frac{d^{m+2}}{dx^{m+2}}P_\ell(x) - 2x\frac{d^{m+1}}{dx^{m+1}}P_\ell(x).$$

Second Term: Expand $-2x\frac{d}{dx}\left[\frac{d^m}{dx^m}P_\ell(x)\right]$:

$$-2x\frac{d}{dx}\left[\frac{d^m}{dx^m}P_\ell(x)\right] = -2x\frac{d^{m+1}}{dx^{m+1}}P_\ell(x).$$

Third Term: The third term remains:

$$\ell(\ell+1)\frac{d^m}{dx^m}P_\ell(x).$$

Substitute these into the equation:

$$(1-x^2)\frac{d^{m+2}}{dx^{m+2}}P_\ell(x) - 4x\frac{d^{m+1}}{dx^{m+1}}P_\ell(x) + \ell(\ell+1)\frac{d^m}{dx^m}P_\ell(x) = 0.$$

Using the definition of $P_\ell^m(x)$:

$$P_\ell^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_\ell(x),$$

we have:

$$\frac{d^m}{dx^m}P_\ell(x) = (1-x^2)^{-m/2}P_\ell^m(x) \tag{62}$$
$$\frac{d^{m+1}}{dx^{m+1}}P_\ell(x) = (1-x^2)^{-(m+1)/2}P_\ell^{m+1}(x) \tag{63}$$
$$\frac{d^{m-1}}{dx^{m-1}}P_\ell(x) = (1-x^2)^{-(m-1)/2}P_\ell^{m-1}(x). \tag{64}$$

Substitute these into the equation:

$$(1-x^2)\cdot(1-x^2)^{-(m+2)/2}P_\ell^{m+2}(x) - 4x(1-x^2)^{-(m+1)/2}P_\ell^{m+1}(x) + \ell(\ell+1)(1-x^2)^{-m/2}P_\ell^m(x) = 0.$$

Factor out the term with the largest power of $(1-x^2)$, which is $(1-x^2)^{m/2}$. Rewrite each term relative to this factor.

First Term:

$$(1-x^2)^{(m/2)-1}P_\ell^{m+2}(x) = (1-x^2)^{m/2}(1-x^2)^{-1}P_\ell^{m+2}(x).$$

Second Term:

$$-4x(1-x^2)^{(m/2)-1/2}P_\ell^{m+1}(x) = -4x(1-x^2)^{m/2}(1-x^2)^{-1/2}P_\ell^{m+1}(x).$$

Third Term:

$$\ell(\ell+1)(1-x^2)^{m/2}P_\ell^m(x) \text{ remains unchanged.}$$

Substitute the rewritten terms back into the equation:

$$(1-x^2)^{m/2}\left[(1-x^2)^{-1}P_\ell^{m+2}(x) - 4x(1-x^2)^{-1/2}P_\ell^{m+1}(x) + \ell(\ell+1)P_\ell^m(x)\right] = 0. \tag{65}$$

Since $(1-x^2)^{m/2} \neq 0$ for $|x| < 1$, divide through by this term:

$$(1-x^2)^{-1}P_\ell^{m+2}(x) - 4x(1-x^2)^{-1/2}P_\ell^{m+1}(x) + \ell(\ell+1)P_\ell^m(x) = 0.$$

Write the terms explicitly:

$$P_\ell^{m+2}(x) \cdot \frac{1}{1-x^2} - P_\ell^{m+1}(x) \cdot \frac{4x}{\sqrt{1-x^2}} + \ell(\ell+1) P_\ell^m(x) = 0.$$

This leads to the recurrence relation:

$$P_\ell^{m+1}(x) + \frac{2mx}{\sqrt{1-x^2}} P_\ell^m(x) + \left[\ell(\ell+1) - m(m-1)\right] P_\ell^{m-1}(x) = 0. \tag{66}$$

Solution 3(b)

The Rodrigues formula for the Legendre polynomials is given by:

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} \left[(x^2-1)^n\right], \tag{67}$$

where n is a non-negative integer. To demonstrate the orthogonality of $P_n(x)$ and to evaluate the integral, we start with:

$$\int_{-1}^{1} P_n(x) P_m(x)\, dx. \tag{68}$$

Substituting the Rodrigues formula for $P_n(x)$ and $P_m(x)$:

$$\int_{-1}^{1} P_n(x) P_m(x)\, dx = \frac{1}{2^n 2^m n! m!} \int_{-1}^{1} \frac{d^n}{dx^n} \left[(x^2-1)^n\right] \frac{d^m}{dx^m} \left[(x^2-1)^m\right] dx. \tag{69}$$

We use the property of integration by parts repeatedly to simplify. Define:

$$u = \frac{d^n}{dx^n} \left[(x^2-1)^n\right], \quad v = \frac{d^m}{dx^m} \left[(x^2-1)^m\right]. \tag{70}$$

Integration by parts gives:

$$\int_{-1}^{1} uv\, dx = \left[u \int v\, dx\right]_{-1}^{1} - \int \left(\frac{du}{dx} \int v\, dx\right) dx. \tag{71}$$

The boundary terms vanish, and for $n \neq m$, the integrals are zero due to orthogonality. Thus:

$$\int_{-1}^{1} P_n(x) P_m(x)\, dx = 0, \quad n \neq m. \tag{72}$$

For $n = m$, the integral simplifies to:

$$\int_{-1}^{1} [P_n(x)]^2 dx = \frac{1}{(2^n n!)^2} \int_{-1}^{1} \left[\frac{d^n}{dx^n}(x^2-1)^n \right]^2 dx. \tag{73}$$

Next, compute $\frac{d^n}{dx^n}(x^2-1)^n$. Using the general formula for differentiation:

$$\frac{d^n}{dx^n}(x^2-1)^n = n! \sum_{k=0}^{n} \binom{n}{k} (-1)^k \frac{(2k)!}{(2k-n)!} x^{2k-n}. \tag{74}$$

When squared and integrated, only even powers of x contribute, yielding:

$$\int_{-1}^{1} x^{2k} dx = \begin{cases} \frac{2}{2k+1}, & k \geq 0, \\ 0, & \text{otherwise.} \end{cases} \tag{75}$$

Substituting back and simplifying, the integral evaluates to:

$$\int_{-1}^{1} [P_n(x)]^2 dx = \frac{2}{2n+1}. \tag{76}$$

This confirms the orthogonality and normalization of the Legendre polynomials.

---

4. Consider the radial part of the separated Schrödinger Equation for a charged particle in a central force field:

$$\left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{2\mu}{\hbar^2} \left(E + \frac{e^2}{r} \right) - \frac{\ell(\ell+1)}{r^2} \right] \mathcal{R} = 0. \tag{77}$$

   (a) Substitute $\mathcal{R} = rR$ and, applying the technique of matched asymptotic expansions, derive the asymptotic solution.

   (b) Solve the equation for $\ell = 0$ to obtain the expression for the ground state energy eigenfunction.

Solution 4(a)

Define $\mathcal{R} = rR(r)$, where $R(r)$ is the modified radial wavefunction. Substituting this into the radial equation:

$$\begin{aligned} \frac{d}{dr}\mathcal{R} &= \frac{d}{dr}(rR) = R + r\frac{dR}{dr} \\ \frac{d^2}{dr^2}\mathcal{R} &= \frac{d}{dr}\left(R + r\frac{dR}{dr} \right) \\ &= \frac{dR}{dr} + \frac{dR}{dr} + r\frac{d^2R}{dr^2} \end{aligned}$$

$$= 2\frac{dR}{dr} + r\frac{d^2R}{dr^2}. \tag{78}$$

Substituting into the original equation (77):

$$\begin{aligned}
\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d(rR)}{dr}\right) &= \frac{1}{r^2}\frac{d}{dr}\left(r^2\left(R + r\frac{dR}{dr}\right)\right) \\
\frac{1}{r^2}\frac{d}{dr}\left(r^2R + r^3\frac{dR}{dr}\right) &= \frac{1}{r^2}\left(2rR + r^2\frac{dR}{dr} + 3r^2\frac{dR}{dr} + r^3\frac{d^2R}{dr^2}\right) \\
\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)\mathcal{R} &= \frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} \\
\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2\mu}{\hbar^2}\left(E + \frac{e^2}{r}\right)R - \frac{\ell(\ell+1)}{r^2}R = 0. &\qquad (79)
\end{aligned}$$

Asymptotic Expansion for Large r: For $r \to \infty$, the potential term $\frac{e^2}{r} \to 0$, and the equation simplifies to:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2\mu E}{\hbar^2}R = 0. \tag{80}$$

Assume the asymptotic form $R(r) \sim e^{-\kappa r}$, where $\kappa = \sqrt{-2\mu E}/\hbar$ (assuming $E < 0$):

$$\frac{dR}{dr} = -\kappa e^{-\kappa r}, \tag{81}$$

$$\frac{d^2R}{dr^2} = \kappa^2 e^{-\kappa r}. \tag{82}$$

Substitute into the simplified equation (80):

$$\kappa^2 e^{-\kappa r} - \frac{2}{r}\kappa e^{-\kappa r} + \frac{2\mu E}{\hbar^2}e^{-\kappa r} = 0. \tag{83}$$

As $r \to \infty$, the term $\frac{2}{r}\kappa e^{-\kappa r}$ vanishes, confirming:

$$\kappa = \sqrt{-\frac{2\mu E}{\hbar^2}}. \tag{84}$$

Asymptotic Expansion for Small r: For $r \to 0$, neglect the energy term E, and the equation becomes:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{\ell(\ell+1)}{r^2}R = 0. \tag{85}$$

Assume a power-law solution $R(r) \sim r^s$:

$$\frac{dR}{dr} = sr^{s-1}, \tag{86}$$

$$\frac{d^2R}{dr^2} = s(s-1)r^{s-2}. \tag{87}$$

Substitute:

$$\begin{aligned} s(s-1)r^{s-2} + \frac{2}{r}sr^{s-1} - \frac{\ell(\ell+1)}{r^2}r^s &= 0 \\ s(s-1) + 2s - \ell(\ell+1) &= 0 \\ s(s+1) &= \ell(\ell+1) \\ s = \ell \text{ or } s &= -(\ell+1). \end{aligned} \tag{88}$$

Thus, $R(r) \sim r^\ell$ as $r \to 0$.

Solution 4(b)

For $\ell = 0$, the radial equation (77) simplifies to:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2\mu}{\hbar^2}\left(E + \frac{e^2}{r}\right)R = 0. \tag{89}$$

Substitute $R(r) = e^{-\kappa r}$:

$$\frac{dR}{dr} = -\kappa e^{-\kappa r}, \tag{90}$$

$$\frac{d^2R}{dr^2} = \kappa^2 e^{-\kappa r}. \tag{91}$$

The equation becomes:

$$\begin{aligned} \kappa^2 e^{-\kappa r} - \frac{2\kappa}{r}e^{-\kappa r} + \frac{2\mu}{\hbar^2}\left(E + \frac{e^2}{r}\right)e^{-\kappa r} &= 0 \\ \kappa^2 - \frac{2\kappa}{r} + \frac{2\mu E}{\hbar^2} + \frac{2\mu e^2}{\hbar^2 r} &= 0. \end{aligned} \tag{92}$$

Coefficient of $\frac{1}{r}$: $-2\kappa + \frac{2\mu e^2}{\hbar^2} = 0 \implies \kappa = \frac{\mu e^2}{\hbar^2}$,
Constant term: $\kappa^2 + \frac{2\mu E}{\hbar^2} = 0 \implies E = -\frac{\mu e^4}{2\hbar^2}$.
The ground state energy is:

$$E_0 = -\frac{\mu e^4}{2\hbar^2}. \tag{93}$$

The normalized ground state wavefunction is:

$$R_0(r) = \sqrt{\left(\frac{1}{\pi a_0^3}\right)}e^{-r/a_0}, \quad a_0 = \frac{\hbar^2}{\mu e^2}. \tag{94}$$

---

5. Answer the following questions:

(a) Show that the quantum mechanical wave function for a one-dimensional simple harmonic oscillator in its n-th energy level has the form:

$$\psi(x) = \exp\left(-\frac{x^2}{2}\right) H_n(x), \tag{95}$$

where $H_n(x)$ is the n-th Hermite polynomial.

(b) The generating function for the polynomial is:

$$G(x,h) = e^{2hx-h^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} h^n. \tag{96}$$

(i) Find $H_i(x)$ for $i = 1, 2, 3, 4$.

(ii) Evaluate $\displaystyle\int_{-\infty}^{\infty} e^{-x^2} H_p(x) H_q(x) dx$.

Solution 5(a)

The time-independent Schrödinger equation for a one-dimensional harmonic oscillator is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi = E_n \psi, \tag{97}$$

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

Let us define:

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x, \quad \text{and rewrite as:} \quad \psi(x) = f(\xi)e^{-\xi^2/2}. \tag{98}$$

Substituting $\psi(x)$ into the Schrödinger equation, we have:

$$-\frac{\hbar^2}{2m}\frac{d}{dx^2}\left(f(\xi)e^{-\xi^2/2}\right) + \frac{1}{2}m\omega^2 x^2 f(\xi)e^{-\xi^2/2} = E_n f(\xi)e^{-\xi^2/2}. \tag{99}$$

Using:

$$\frac{d}{dx} = \sqrt{\frac{m\omega}{\hbar}}\frac{d}{d\xi},$$
$$\frac{d^2}{dx^2} = \frac{m\omega}{\hbar}\frac{d^2}{d\xi^2},$$

the equation becomes:

$$\left[-\frac{\hbar\omega}{2}\frac{d^2}{d\xi^2} + \frac{1}{2}\hbar\omega\xi^2\right] f(\xi)e^{-\xi^2/2} = E_n f(\xi)e^{-\xi^2/2}$$
$$-\frac{\hbar\omega}{2}\left(\frac{d^2 f}{d\xi^2} - 2\xi\frac{df}{d\xi} + \xi^2 f\right) + \frac{1}{2}\hbar\omega\xi^2 f = E_n f$$

$$\frac{d^2 f}{d\xi^2} - 2\xi\frac{df}{d\xi} + \left[2n - \xi^2\right] f = 0. \tag{100}$$

This is the Hermite differential equation, whose solutions are the Hermite polynomials:

$$f(\xi) = H_n(\xi), \tag{101}$$

$$\psi(x) = e^{-\xi^2/2} H_n(\xi), \tag{102}$$

where $\xi = \sqrt{\frac{m\omega}{\hbar}} x$. Thus:

$$\psi(x) = e^{-x^2/2} H_n(x).$$

Solution 5(b)(i)

The generating function for Hermite polynomials is:

$$G(x,h) = e^{2hx - h^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} h^n. \tag{103}$$

Expand $G(x,h)$ to compute $H_n(x)$ for $n = 0, 1, 2, 3, 4$:

- For $n = 0$:

$$H_0(x) = 1. \tag{104}$$

- For $n = 1$:

$$H_1(x) = \left.\frac{\partial G(x,h)}{\partial h}\right|_{h=0} = 2x. \tag{105}$$

- For $n = 2$:

$$H_2(x) = \left.\frac{\partial^2 G(x,h)}{\partial h^2}\right|_{h=0} = 4x^2 - 2. \tag{106}$$

- For $n = 3$:

$$H_3(x) = \left.\frac{\partial^3 G(x,h)}{\partial h^3}\right|_{h=0} = 8x^3 - 12x. \tag{107}$$

- For $n = 4$:

$$H_4(x) = \left.\frac{\partial^4 G(x,h)}{\partial h^4}\right|_{h=0} = 16x^4 - 48x^2 + 12. \tag{108}$$

Thus:

$$H_0(x) = 1, \quad H_1(x) = 2x, \quad H_2(x) = 4x^2 - 2, \tag{109}$$
$$H_3(x) = 8x^3 - 12x, \quad H_4(x) = 16x^4 - 48x^2 + 12. \tag{110}$$

Solution 5(b)(ii)

The orthogonality relation for Hermite polynomials is:

$$\int_{-\infty}^{\infty} e^{-x^2} H_p(x) H_q(x) dx = \delta_{pq} \sqrt{\pi} 2^p p!. \tag{111}$$

Start with the generating function:

$$G(x,h) = e^{2hx-h^2}.$$

Multiply $G(x,h)$ by $G(x,h')$ and integrate over x:

$$\begin{aligned}
\int_{-\infty}^{\infty} e^{-x^2} G(x,h) G(x,h') dx &= \int_{-\infty}^{\infty} e^{-x^2} e^{2hx-h^2} e^{2h'x-h'^2} dx \\
&= \int_{-\infty}^{\infty} e^{-x^2} e^{2(h+h')x-(h^2+h'^2)} dx \\
&= e^{-(h^2+h'^2)} \int_{-\infty}^{\infty} e^{-x^2+2(h+h')x} dx \\
&= e^{-(h^2+h'^2)} \int_{-\infty}^{\infty} e^{-(x-(h+h'))^2+(h+h')^2} \\
&= e^{-(h^2+h'^2)+(h+h')^2} \int_{-\infty}^{\infty} e^{-(x-(h+h'))^2} dx \qquad (112) \\
&= \sqrt{\pi} e^{2hh'}. \qquad (113)
\end{aligned}$$

Expanding $e^{2hh'}$ as a double power series:

$$e^{2hh'} = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \frac{H_p(x)}{p!} \frac{H_q(x)}{q!} h^p h'^q.$$

Equating coefficients of $h^p h'^q$:

$$\int_{-\infty}^{\infty} e^{-x^2} H_p(x) H_q(x) dx = \delta_{pq} \sqrt{\pi} 2^p p!. \tag{114}$$

Thus, the orthogonality relation is proved.

---

6. Consider a particle executing simple harmonic motion $x = a\cos\omega t$ on $(-a, a)$ along the x-axis.
   (a) Find the probability density function $f(x)$ for the position x.
   (b) Sketch the probability density function $f(x)$.
   (c) Find the average and the standard deviation of x.

Solution 6(a)

The probability density function $f(x)$ is proportional to the time the particle spends near position x. Since the particle slows down as it approaches the turning points ($x = \pm a$), the probability density is higher near these points.

The equation of motion is:

$$\begin{aligned} x &= a\cos\omega t \\ \therefore t &= \frac{1}{\omega}\cos^{-1}\left(\frac{x}{a}\right). \end{aligned} \tag{115}$$

The velocity is:

$$v = \frac{dx}{dt} = -a\omega\sin(\omega t). \tag{116}$$

Using the trigonometric identity $\sin^2(\omega t) = 1 - \cos^2(\omega t)$ and substituting $x = a\cos(\omega t)$, we have:

$$\begin{aligned} \sin^2(\omega t) &= 1 - \frac{x^2}{a^2} \\ \sin(\omega t) &= \pm\sqrt{1 - \frac{x^2}{a^2}}. \end{aligned} \tag{117}$$

Substitute into $v = -a\omega\sin(\omega t)$:

$$v = -\omega\sqrt{a^2 - x^2}. \tag{118}$$

The time spent near position x is inversely proportional to the magnitude of the velocity:

$$\Delta t \propto \frac{1}{|v|}.$$

Thus, the probability density function is proportional to:

$$f(x) \propto \frac{1}{|v|} = \frac{1}{\omega\sqrt{a^2 - x^2}}.$$

We now normalize $f(x)$ over the interval $(-a, a)$. Define the normalization constant N:

$$\int_{-a}^{a} f(x)dx = 1.$$

$$\int_{-a}^{a} \frac{1}{N\sqrt{a^2 - x^2}}dx = 1$$

$$\frac{1}{N}\int_{-a}^{a} \frac{1}{\sqrt{a^2 - x^2}}dx = 1. \tag{119}$$

The integral $\int_{-a}^{a} \frac{1}{\sqrt{a^2 - x^2}}dx$ is a standard result for a semicircular arc:

$$\int_{-a}^{a} \frac{1}{\sqrt{a^2 - x^2}}dx = \pi$$

$$\frac{1}{N}\pi = 1 \implies N = \pi. \tag{120}$$

The normalized probability density function is:

$$f(x) = \frac{1}{\pi\sqrt{a^2 - x^2}}, \quad x \in (-a, a). \tag{121}$$

Solution 6(b)

The function $f(x)$ is symmetric about $x = 0$ and diverges near $x = \pm a$. Its graph has the shape of an inverse square-root curve centered at the origin.

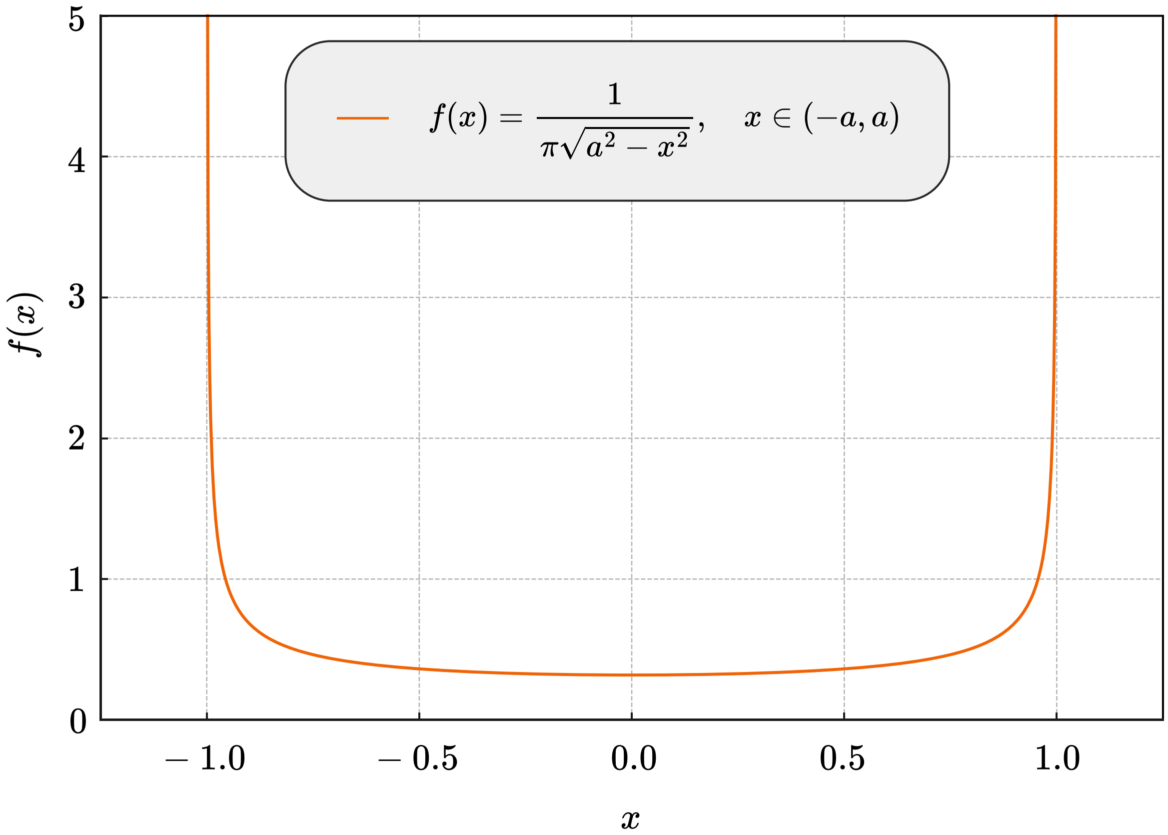

Figure 1: Probability density function $f(x)$ for the particle's position.

Solution 6(c)

The mean $\langle x \rangle$ is given by:

$$\langle x \rangle = \int_{-a}^{a} x f(x) dx = \int_{-a}^{a} \frac{x}{\pi\sqrt{a^2 - x^2}} dx. \tag{122}$$

The integrand $\frac{x}{\sqrt{a^2 - x^2}}$ is an odd function, since:

$$\frac{-x}{\sqrt{a^2 - (-x)^2}} = -\frac{x}{\sqrt{a^2 - x^2}}.$$

Integrating an odd function over symmetric limits yields zero:

$$\langle x \rangle = 0.$$

The variance is defined as:

$$\text{Var}(x) = \langle x^2 \rangle - \langle x \rangle^2.$$

Since $\langle x \rangle = 0$, it simplifies to:

$$\text{Var}(x) = \langle x^2 \rangle.$$

The expectation value $\langle x^2 \rangle$ is:

$$\langle x^2 \rangle = \int_{-a}^{a} x^2 f(x) dx = \int_{-a}^{a} \frac{x^2}{\pi\sqrt{a^2 - x^2}} dx.$$

Substitute $x = a \sin\theta$, so:

$$dx = a\cos\theta \, d\theta, \quad \sqrt{a^2 - x^2} = a\cos\theta.$$

The limits of integration change:

$$x = -a \implies \theta = -\frac{\pi}{2}, \quad x = a \implies \theta = \frac{\pi}{2}.$$

Substituting into the integral:

$$\langle x^2 \rangle = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} \frac{a^2 \sin^2\theta}{a\cos\theta} a\cos\theta \, d\theta$$

$$\langle x^2 \rangle = \frac{a^2}{\pi} \int_{-\pi/2}^{\pi/2} \sin^2\theta \, d\theta.$$

Using the identity $\sin^2\theta = \frac{1}{2}(1 - \cos(2\theta))$:

$$\begin{aligned}
\langle x^2 \rangle &= \frac{a^2}{\pi} \int_{-\pi/2}^{\pi/2} \frac{1}{2}(1 - \cos(2\theta)) \, d\theta. \\
&= \frac{a^2}{\pi} \left[\frac{1}{2} \int_{-\pi/2}^{\pi/2} 1 \, d\theta - \frac{1}{2} \int_{-\pi/2}^{\pi/2} \cos(2\theta) \, d\theta \right]. \\
&= \frac{a^2}{\pi} \left[\frac{1}{2}\pi - \frac{1}{2} \frac{\sin(2\theta)}{2} \Big|_{-\pi/2}^{\pi/2} \right] \\
&= \frac{a^2}{\pi} \left[\frac{1}{2}\pi - \frac{\sin(\pi)}{2} - \frac{\sin(-\pi)}{2} \right] \\
&= \frac{a^2}{\pi} \left[\frac{1}{2}\pi - 0 \right] \\
&= \frac{a^2}{2}.
\end{aligned} \tag{123}$$

The standard deviation is:

$$\sigma_x = \sqrt{\langle x^2 \rangle} = \sqrt{\frac{a^2}{2}} = \frac{a}{\sqrt{2}}. \tag{124}$$

7. If ψ_1 and ψ_2 are two solutions of the time-dependent Schrödinger equation, then for real V, prove that:

$$\frac{\partial(\psi_1^*\psi_2)}{\partial t} + \frac{\hbar}{2mi}\nabla \cdot \left[\psi_1^*\nabla\psi_2 - (\nabla\psi_1^*)\psi_2\right] = 0. \tag{125}$$

Solution 7

The time-dependent Schrödinger equations for ψ_1 and ψ_2 are:

$$i\hbar\frac{\partial\psi_1}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi_1 + V\psi_1, \tag{126}$$

$$i\hbar\frac{\partial\psi_2}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi_2 + V\psi_2. \tag{127}$$

Take the complex conjugate of (126):

$$-i\hbar\frac{\partial\psi_1^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi_1^* + V\psi_1^*. \tag{128}$$

Compute the time derivative of $\psi_1^*\psi_2$:

$$\frac{\partial(\psi_1^*\psi_2)}{\partial t} = \psi_1^*\frac{\partial\psi_2}{\partial t} + \left(\frac{\partial\psi_1^*}{\partial t}\right)\psi_2. \tag{129}$$

Substitute $\frac{\partial\psi_2}{\partial t}$ from (127) and $\frac{\partial\psi_1^*}{\partial t}$ from the conjugate of (126):

$$\frac{\partial(\psi_1^*\psi_2)}{\partial t} = \psi_1^*\left(-\frac{i\hbar}{2m}\nabla^2\psi_2 + \frac{i}{\hbar}V\psi_2\right) + \left(-\frac{i\hbar}{2m}\nabla^2\psi_1^* + \frac{i}{\hbar}V\psi_1^*\right)\psi_2$$

$$\frac{\partial(\psi_1^*\psi_2)}{\partial t} = -\frac{i\hbar}{2m}\left(\psi_1^*\nabla^2\psi_2 - (\nabla^2\psi_1^*)\psi_2\right). \tag{130}$$

Since V is real, the potential terms cancel.

Next, compute the divergence term:

$$\nabla \cdot \left[\psi_1^*\nabla\psi_2 - (\nabla\psi_1^*)\psi_2\right] = \nabla \cdot (\psi_1^*\nabla\psi_2) - \nabla \cdot ((\nabla\psi_1^*)\psi_2). \tag{131}$$

Using the product rule for divergence:

$$\nabla \cdot (\psi_1^*\nabla\psi_2) = (\nabla\psi_1^*)\cdot(\nabla\psi_2) + \psi_1^*\nabla^2\psi_2$$

$$\nabla \cdot ((\nabla\psi_1^*)\psi_2) = (\nabla^2\psi_1^*)\psi_2 + (\nabla\psi_1^*)\cdot(\nabla\psi_2)$$

$$\nabla \cdot \left[\psi_1^*\nabla\psi_2 - (\nabla\psi_1^*)\psi_2\right] = \psi_1^*\nabla^2\psi_2 - (\nabla^2\psi_1^*)\psi_2. \tag{132}$$

Substitute the divergence term into the original expression:

$$\frac{\partial(\psi_1^*\psi_2)}{\partial t} + \frac{\hbar}{2mi}\nabla \cdot \Big[\psi_1^*\nabla\psi_2 - (\nabla\psi_1^*)\psi_2\Big]. \tag{133}$$

Using the expressions derived:

$$\begin{aligned}
\frac{\partial(\psi_1^*\psi_2)}{\partial t} &= -\frac{i\hbar}{2m}\Big(\psi_1^*\nabla^2\psi_2 - (\nabla^2\psi_1^*)\psi_2\Big) \\
\frac{\hbar}{2mi}\nabla \cdot \Big[\psi_1^*\nabla\psi_2 - (\nabla\psi_1^*)\psi_2\Big] &= \frac{\hbar}{2mi}\Big(\psi_1^*\nabla^2\psi_2 - (\nabla^2\psi_1^*)\psi_2\Big) \\
\frac{\partial(\psi_1^*\psi_2)}{\partial t} + \frac{\hbar}{2mi}\nabla \cdot \Big[\psi_1^*\nabla\psi_2 - (\nabla\psi_1^*)\psi_2\Big] &= 0. \qquad (134)
\end{aligned}$$

---

8. Consider a linear harmonic oscillator. Answer the following questions:
   (a) Apply the Bohr postulate to obtain the quantum energies of this system.
   (b) From the Hamilton-Jacobi equation for this system, derive the Schrödinger equation stating all necessary conditions.
   (c) State and apply the Heisenberg quantization conditions to derive the expression for the ground state energy E_0, general expressions for E_n, and expressions for q's and p's.
   (d) Show that the expectation value for the potential energy of the linear harmonic oscillator is $\langle V\rangle_n = \frac{1}{2}E_n$.
   (e) Find $(\Delta x)^2$ and $(\Delta p)^2$, and show that the minimum possible value of the uncertainty product is $\frac{1}{2}\hbar$.

Solution 8(a)

The Bohr quantization postulate states that the action integral over one complete cycle is quantized:

$$\oint p\,dq = nh, \quad n = 0, 1, 2, \ldots,$$

where p is the momentum and q is the position.

For a harmonic oscillator, the Hamiltonian is:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 = E \tag{135}$$

$$p = \pm\sqrt{2m(E - \frac{1}{2}m\omega^2 q^2)}. \tag{136}$$

The action integral becomes:

$$\oint p\,dq = 2\int_{-q_{\max}}^{q_{\max}} \sqrt{2m(E - \frac{1}{2}m\omega^2 q^2)}\,dq, \tag{137}$$

where $q_{\max} = \sqrt{\frac{2E}{m\omega^2}}$.
Change variables:

$$q = q_{\max}\sin\theta, \quad dq = q_{\max}\cos\theta\,d\theta.$$

The limits change from $q = -q_{\max}$ to $q = q_{\max}$ corresponding to $\theta = -\pi/2$ to $\theta = \pi/2$. Substitute:

$$\begin{aligned}\oint p\,dq &= 2\int_{-\pi/2}^{\pi/2} \sqrt{2m\left(E - \frac{1}{2}m\omega^2 q_{\max}^2\sin^2\theta\right)}q_{\max}\cos\theta\,d\theta \\ &= 2\sqrt{2mE}\int_{-\pi/2}^{\pi/2} \sqrt{1-\sin^2\theta}q_{\max}\cos\theta\,d\theta. \end{aligned}\tag{138}$$

Evaluate:

$$\oint p\,dq = 2E\frac{\pi}{\omega}. \tag{139}$$

Quantize:

$$2E\frac{\pi}{\omega} = nh, \tag{140}$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right). \tag{141}$$

Solution 8(b)

The classical Hamilton-Jacobi equation for the harmonic oscillator:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 = E. \tag{142}$$

Substitute $p = \frac{\partial S}{\partial q}$:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + \frac{1}{2}m\omega^2 q^2 = 0. \tag{143}$$

Let $S(q,t) = W(q) - Et$, where $W(q)$ is the spatial part:

$$\frac{1}{2m}\left(\frac{dW}{dq}\right)^2 + \frac{1}{2}m\omega^2 q^2 = E. \tag{144}$$

Quantize using $\hat{p} = -i\hbar\frac{\partial}{\partial q}$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q^2} + \frac{1}{2}m\omega^2 q^2\psi = E\psi. \tag{145}$$

This is the time-independent Schrödinger equation.

Solution 8(c)

The Heisenberg quantization condition is:

$$[q,p] = i\hbar. \tag{146}$$

Define the ladder operators $\hat{a}$ and $\hat{a}^\dagger$ as:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(q + \frac{ip}{m\omega}\right), \tag{147}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(q - \frac{ip}{m\omega}\right). \tag{148}$$

To verify the commutator:

$$\begin{aligned}[\hat{a},\hat{a}^\dagger] &= \sqrt{\frac{m\omega}{2\hbar}}\left[q + \frac{ip}{m\omega}, q - \frac{ip}{m\omega}\right] \\ &= \frac{m\omega}{2\hbar}\left([q,q] - \frac{i}{m\omega}[q,p] + \frac{i}{m\omega}[p,q] - \frac{1}{(m\omega)^2}[p,p]\right).\end{aligned} \tag{149}$$

Since $[q,q] = 0$, $[p,p] = 0$, and $[q,p] = i\hbar$:

$$\begin{aligned}[\hat{a},\hat{a}^\dagger] &= \frac{m\omega}{2\hbar}\left(0 - \frac{i}{m\omega}(i\hbar) + \frac{i}{m\omega}(i\hbar) - 0\right) \\ [\hat{a},\hat{a}^\dagger] &= 1.\end{aligned} \tag{150}$$

Rearranging the definitions of $\hat{a}$ and $\hat{a}^\dagger$:

$$q = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger), \tag{151}$$

$$p = -i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a} - \hat{a}^\dagger). \tag{152}$$

Solution 8(d)

Substitute q and p into the Hamiltonian:

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

Compute q^2 and p^2:

$$\begin{aligned} q^2 &= \frac{\hbar}{2m\omega}(\hat{a} + \hat{a}^\dagger)^2, \\ p^2 &= -\frac{\hbar m\omega}{2}(\hat{a} - \hat{a}^\dagger)^2. \end{aligned} \tag{153}$$

Substitute into H:

$$\begin{aligned} H &= \frac{1}{2m}\left(-\frac{\hbar m\omega}{2}(\hat{a} - \hat{a}^\dagger)^2\right) + \frac{1}{2}m\omega^2\left(\frac{\hbar}{2m\omega}(\hat{a} + \hat{a}^\dagger)^2\right) \\ H &= \frac{\hbar\omega}{2}\left[\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger + \frac{1}{2}\right]. \end{aligned}$$

Using $[\hat{a}, \hat{a}^\dagger] = 1$:

$$\begin{aligned} \hat{a}\hat{a}^\dagger &= \hat{a}^\dagger\hat{a} + 1 \\ H &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right). \end{aligned} \tag{154}$$

The number operator is defined as:

$$\hat{N} = \hat{a}^\dagger\hat{a}.$$

The Hamiltonian becomes:

$$H = \hbar\omega\left(\hat{N} + \frac{1}{2}\right).$$

The eigenvalues of $\hat{N}$ are $n = 0, 1, 2, \ldots$, so the energy levels are:

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

For $n = 0$, the energy is:

$$E_0 = \frac{1}{2}\hbar\omega.$$

The potential energy of a harmonic oscillator is:

$$V(q) = \frac{1}{2}m\omega^2 q^2. \tag{155}$$

The total Hamiltonian of the harmonic oscillator is:

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

In quantum mechanics, the total energy E_n of the n-th eigenstate is:

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

The expectation value of the Hamiltonian is:

$$\langle H \rangle_n = E_n. \tag{156}$$

The Hamiltonian consists of the kinetic energy $T = \dfrac{p^2}{2m}$ and the potential energy $V(q)$:

$$H = T + V(q).$$

By the virial theorem, for a harmonic oscillator in a stationary state, the expectation values of T and V are equal:

$$\langle T \rangle_n = \langle V \rangle_n.$$

Thus:

$$\begin{aligned}
\langle H \rangle_n &= \langle T \rangle_n + \langle V \rangle_n = 2\langle V \rangle_n \\
\langle V \rangle_n &= \frac{1}{2}\langle H \rangle_n \\
&= \frac{1}{2}E_n.
\end{aligned} \tag{157}$$

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

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

Solution 8(e)

For the ground state, $\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}$.

The uncertainties are:

$$\begin{aligned}
(\Delta x)^2 &= \langle x^2 \rangle - \langle x \rangle^2 = \frac{\hbar}{2m\omega} \\
(\Delta p)^2 &= \langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar m\omega}{2}.
\end{aligned} \tag{158}$$

The uncertainty product is:

$$\Delta x \Delta p = \sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{\hbar m\omega}{2}} = \frac{\hbar}{2}. \tag{159}$$

This satisfies the uncertainty principle:

$$\Delta x \Delta p \geq \frac{\hbar}{2}.$$

---

9. Solve the two-body problem using the Hamilton-Jacobi equation.

Solution 9

Let the position vectors of the masses be $\mathbf{r}_1$ and $\mathbf{r}_2$. Define the center-of-mass coordinate $\mathbf{R}$ and the relative coordinate $\mathbf{r}$ as:

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2. \tag{160}$$

The total kinetic energy T of the system can be written as:

$$T = \frac{1}{2}m_1\dot{\mathbf{r}}_1^2 + \frac{1}{2}m_2\dot{\mathbf{r}}_2^2. \tag{161}$$

Substitute:

$$\mathbf{r}_1 = \mathbf{R} + \frac{m_2}{m_1 + m_2}\mathbf{r}, \quad \mathbf{r}_2 = \mathbf{R} - \frac{m_1}{m_1 + m_2}\mathbf{r}.$$

Differentiate:

$$\dot{\mathbf{r}}_1 = \dot{\mathbf{R}} + \frac{m_2}{m_1 + m_2}\dot{\mathbf{r}}, \quad \dot{\mathbf{r}}_2 = \dot{\mathbf{R}} - \frac{m_1}{m_1 + m_2}\dot{\mathbf{r}}.$$

Substitute into T:

$$T = \frac{1}{2}(m_1 + m_2)\dot{\mathbf{R}}^2 + \frac{1}{2}\mu\dot{\mathbf{r}}^2, \tag{162}$$

where $\mu = \dfrac{m_1 m_2}{m_1 + m_2}$ is the reduced mass.
The potential energy V depends only on the relative distance $r = |\mathbf{r}|$:

$$V = V(r).$$

The total Hamiltonian becomes:

$$H = \frac{1}{2}(m_1 + m_2)\dot{\mathbf{R}}^2 + \frac{1}{2}\mu\dot{\mathbf{r}}^2 + V(r).$$

The Hamilton-Jacobi equation is:

$$\frac{\partial S}{\partial t} + H\left(\mathbf{R}, \mathbf{r}, \frac{\partial S}{\partial \mathbf{R}}, \frac{\partial S}{\partial \mathbf{r}}\right) = 0.$$

Substitute H:

$$\frac{\partial S}{\partial t} + \frac{1}{2(m_1 + m_2)} \left(\frac{\partial S}{\partial \mathbf{R}} \right)^2 + \frac{1}{2\mu} \left(\frac{\partial S}{\partial \mathbf{r}} \right)^2 + V(r) = 0.$$

Let the action S separate as:

$$S = S_{\text{CM}}(\mathbf{R}, t) + S_{\text{rel}}(\mathbf{r}, t). \tag{163}$$

Substitute into the Hamilton-Jacobi equation:

$$\frac{\partial S_{\text{CM}}}{\partial t} + \frac{1}{2(m_1 + m_2)} \left(\frac{\partial S_{\text{CM}}}{\partial \mathbf{R}} \right)^2 + \frac{\partial S_{\text{rel}}}{\partial t} + \frac{1}{2\mu} \left(\frac{\partial S_{\text{rel}}}{\partial \mathbf{r}} \right)^2 + V(r) = 0.$$

Separate variables:

$$\begin{aligned} \frac{\partial S_{\text{CM}}}{\partial t} + \frac{1}{2(m_1 + m_2)} \left(\frac{\partial S_{\text{CM}}}{\partial \mathbf{R}} \right)^2 &= E_{\text{CM}} \\ \frac{\partial S_{\text{rel}}}{\partial t} + \frac{1}{2\mu} \left(\frac{\partial S_{\text{rel}}}{\partial \mathbf{r}} \right)^2 + V(r) &= E_{\text{rel}}, \end{aligned} \tag{164}$$

where $E = E_{\text{CM}} + E_{\text{rel}}$.

The equation for S_{CM} is:

$$\frac{\partial S_{\text{CM}}}{\partial t} + \frac{1}{2(m_1 + m_2)} \left(\frac{\partial S_{\text{CM}}}{\partial \mathbf{R}} \right)^2 = E_{\text{CM}}. \tag{165}$$

Assume $S_{\text{CM}} = -E_{\text{CM}} t + \mathbf{P}_{\text{CM}} \cdot \mathbf{R}$, where $\mathbf{P}_{\text{CM}}$ is the total momentum:

$$\begin{aligned} \frac{\partial S_{\text{CM}}}{\partial t} = -E_{\text{CM}}, \quad \frac{\partial S_{\text{CM}}}{\partial \mathbf{R}} = \mathbf{P}_{\text{CM}}, \\ \therefore E_{\text{CM}} = \frac{\mathbf{P}_{\text{CM}}^2}{2(m_1 + m_2)}. \end{aligned} \tag{166}$$

The equation for S_{rel} is:

$$\frac{\partial S_{\text{rel}}}{\partial t} + \frac{1}{2\mu} \left(\frac{\partial S_{\text{rel}}}{\partial \mathbf{r}} \right)^2 + V(r) = E_{\text{rel}}. \tag{167}$$

Assume $S_{\text{rel}} = -E_{\text{rel}} t + W(\mathbf{r})$, where $W(\mathbf{r})$ satisfies:

$$\frac{1}{2\mu} (\nabla W)^2 + V(r) = E_{\text{rel}}.$$

In spherical coordinates, assume $W(\mathbf{r}) = W(r, \theta, \phi) = W_r(r) + W_\Omega(\theta, \phi)$. The angular part corresponds to the conservation of angular momentum:

$$W_\Omega(\theta, \phi) \sim m_\phi \phi + \ell(\ell + 1)\theta.$$

The radial part reduces to:

$$\frac{1}{2\mu}\left(\frac{dW_r}{dr}\right)^2 + V_{\text{eff}}(r) = E_{\text{rel}},$$

where:

$$V_{\text{eff}}(r) = V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}. \tag{168}$$

This equation determines the radial motion.

The total action is:

$$S = \mathbf{P}_{\text{CM}} \cdot \mathbf{R} - E_{\text{CM}}t + W_r(r) + W_\Omega(\theta,\phi) - E_{\text{rel}}t. \tag{169}$$

This solution fully describes the motion of the two-body system using the Hamilton-Jacobi formalism.