CSCD94 A3

1. Schrodinger Equation

a) Separation of Variables

We start with the time-dependent Schrödinger equation in one dimension:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t)$$

Assume the wave function can be separated as $\Psi(x,t) = \psi(x)\phi(t)$. Substituting this into the Schrödinger equation:

$$i\hbar\cdot\psi(x)\frac{d\phi(t)}{dt} = \left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)\right)\phi(t)$$

Divide both sides by $\psi(x)\phi(t)$:

$$i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = \frac{1}{\psi(x)}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)\right)$$

The left-hand side depends only on t, and the right-hand side depends only on x. For this equality to hold for all x and t, both sides must be equal to a constant, which we denote as E (the separation constant).

b): Time-Independent Schrödinger Equation and Time-Dependent Equation

From the separation of variables, we obtain two ordinary differential equations:

1. **Time-dependent equation**:

$$i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = E$$

Rearranging:

$$\frac{d\phi(t)}{dt} = -\frac{iE}{\hbar}\phi(t)$$

2. **Time-independent Schrödinger equation (TISE)**:

$$\frac{1}{\psi(x)}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)\right) = E$$

Rearranging:

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

c): Solving the Time-Dependent Equation

The time-dependent equation is:

$$\frac{d\phi(t)}{dt} = -\frac{iE}{\hbar}\phi(t)$$

This is a first-order linear differential equation. To solve it, we separate variables and integrate:

$$\int \frac{1}{\phi(t)} d\phi(t) = -\frac{iE}{\hbar}\int dt$$

Integrating both sides:

$$\ln \phi(t) = -\frac{iE}{\hbar}t + C$$

Exponentiating both sides to solve for $\phi(t)$:

$$\phi(t) = e^{C}e^{-\frac{iE}{\hbar}t}$$

Let $e^C = A$ (a constant), so:

$$\phi(t) = Ae^{-\frac{iE}{\hbar}t}$$

The constant A can be absorbed into the spatial part $\psi(x)$ when reconstructing the full wave function $\Psi(x,t) = \psi(x)\phi(t)$. Thus, the solution is:

$$\phi(t) = e^{-\frac{iE}{\hbar}t}$$

2. Particle in a box or the infinite well potential

a): General Solution to the TISE

For the infinite potential well defined by:

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{for } x < 0 \text{ or } x > L \end{cases}$$

The Time-Independent Schrödinger Equation (TISE) inside the well ($0 < x < L$) reduces to:

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

Rearranging:

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

where $k^2 = \frac{2mE}{\hbar^2}$. The general solution is:

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

b): Applying Boundary Conditions

Boundary conditions: $\psi(0) = 0$ and $\psi(L) = 0$.

1. At $x = 0$:

$$\psi(0) = A\sin(0) + B\cos(0) = B = 0$$

Thus, $\psi(x) = A\sin(kx)$.

2. At $x = L$:

$$\psi(L) = A\sin(kL) = 0 \implies kL = n\pi \quad (n = 1, 2, 3, \dots)$$

Quantized k_n and energy E_n:

$$k_n = \frac{n\pi}{L}, \quad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Final solution:

$$\psi_n(x) = A\sin\left(\frac{n\pi x}{L}\right)$$

c): Important Observation

The solution reveals **quantization**:

- Discrete energy levels E_n and wave numbers k_n.
- Quantum number n defines allowed states.
- Standing waves with nodes at boundaries.

3. Classic Harmonic Oscillator

a): Pendulum Equation of Motion

For small angles θ, $\theta \approx \sin(\theta)$, the equation of motion is:

$$\ddot{\theta} + \frac{g}{l}\theta = 0.$$

Here, $\omega = \sqrt{\frac{g}{l}}$.

b): General Solution

The general solution is:

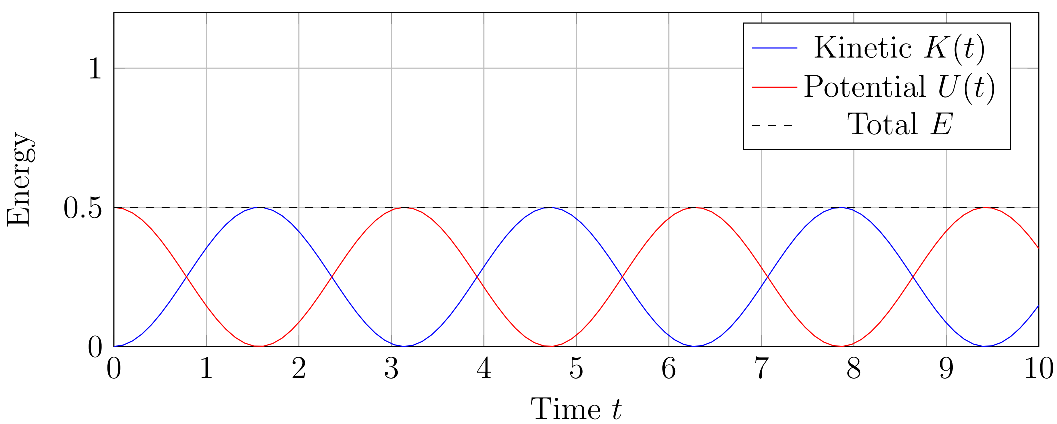
$$\theta(t) = \Theta \cos(\omega t + \phi),$$

where $\Theta = \sqrt{A^2 + B^2}$ is the amplitude and $\phi = \tan^{-1}(-B/A)$ the phase. The 'most' general solution can assume $\phi = 0$ which means our general solution becomes $\theta(t) = \Theta \cos(\omega t)$

c): Energy and Phase-Space

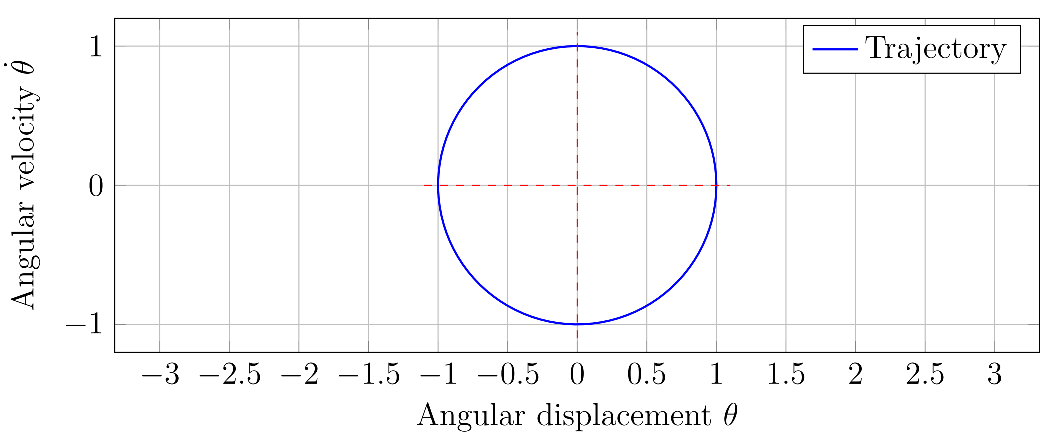
- **Energy vs Time**:

Energy vs. Time for $\theta_0 = 1$, $\omega = 1$, $mgL = 1$



- **Phase-Space Diagram**:

Phase-Space Diagram ($\theta_0 = 1$, $\omega = 1$)



4. Quantum Harmonic Oscillator

a) Hamiltonian

$$\hat{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

where p is the momentum operator, and ω is the angular frequency.

b): Time-Independent Schrödinger Equation

Substituting the Hamiltonian into the TISE $\hat{H}\psi = E\psi$:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right]\psi(x) = E\psi(x).$$

The eigenfunctions $\psi_n(x)$ involve Hermite polynomials H_n:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right),$$

where H_n are the Hermite polynomials defined by:

$$H_n(z) = (-1)^n e^{z^2}\frac{d^n}{dz^n}\left(e^{-z^2}\right).$$

c): Code

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.special import hermite
from matplotlib.gridspec import GridSpec
import math

# Set up the figure and subplots
fig = plt.figure(figsize=(14, 8))
gs = GridSpec(2, 1, height_ratios=[1, 1])

ax1 = fig.add_subplot(gs[0])  # Wavefunctions
ax2 = fig.add_subplot(gs[1])  # Probability densities

# Parameters
x = np.linspace(-4, 4, 500)
n_values = range(8)  # n = 0 to 7
colors = plt.cm.viridis(np.linspace(0, 1, len(n_values)))  # Color gradient

# Common function to calculate QHO states
def qho_state(n, x, m=1.0, omega=1.0, hbar=1.0):
    coeff = 1 / np.sqrt(2**n * math.factorial(n)) * (m * omega / (np.pi * hbar))**(0.25)
    exponent = np.exp(-m * omega * x**2 / (2 * hbar))
    z = np.sqrt(m * omega / hbar) * x
```

```
    H_n = hermite(n)(z)
    return coeff * exponent * H_n

# Plot wavefunctions and probability densities
for n, color in zip(n_values, colors):
    psi = qho_state(n, x)
    prob = psi**2

    # Offset each wavefunction for clarity
    y_offset = 1.5 * n
    ax1.plot(x, psi + y_offset, color=color, label=f'n={n}')
    ax1.fill_between(x, y_offset, psi + y_offset, color=color, alpha=0.2)

    # Plot probability densities
    ax2.plot(x, prob, color=color, label=f'n={n}')
    ax2.fill_between(x, 0, prob, color=color, alpha=0.2)

# Format wavefunction plot
ax1.set_title('Wavefunctions $\psi_n(x)$ for QHO (n=0 to 7)')
ax1.set_ylabel('$\psi_n(x)$ (offset)')
ax1.set_yticks([1.5 * n for n in n_values])
ax1.set_yticklabels([f'n={n}' for n in n_values])
ax1.axhline(0, color='black', linewidth=0.5, linestyle='--')
ax1.grid(True, alpha=0.3)

# Format probability density plot
ax2.set_title('Probability Densities $|\psi_n(x)|^2$ for QHO (n=0 to 7)')
ax2.set_xlabel('Position $x$')
ax2.set_ylabel('$|\psi_n(x)|^2$')
ax2.grid(True, alpha=0.3)
ax2.set_ylim(0, 0.6)

plt.tight_layout()
plt.show()
```

5. Tunneling

(a) TISE in Each Region

For the potential:

$$V(x) = \begin{cases} 0 & x < 0 \quad \text{(Region I)} \\ V_0 & 0 \leq x \leq a \quad \text{(Region II)} \\ 0 & x > a \quad \text{(Region III)} \end{cases}$$

- **Region I & III** ($V(x) = 0$):

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

- **Region II** ($V(x) = V_0 > E$):

$$\frac{d^2\psi}{dx^2} - \kappa^2\psi = 0, \quad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

(b) General Wave Functions

- **Region I**:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$$

  (Incident + reflected waves)

- **Region II**:

$$\psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x}$$

  (Exponentially decaying/growing)

- **Region III**:

$$\psi_{III}(x) = Fe^{ikx}$$

  (Transmitted wave only)

(c) Boundary Conditions

At $x = 0$:

$$\begin{cases} A + B = C + D \\ ik(A - B) = \kappa(C - D) \end{cases}$$

At $x = a$:

$$\begin{cases} Ce^{\kappa a} + De^{-\kappa a} = Fe^{ika} \\ \kappa(Ce^{\kappa a} - De^{-\kappa a}) = ikFe^{ika} \end{cases}$$

(d) Transmission Coefficient T

From part c),

$$C = \frac{(\kappa + ik)}{2\kappa} F e^{ika - \kappa a}, \quad D = \frac{(\kappa - ik)}{2\kappa} F e^{ika + \kappa a}$$

$$A = \frac{F}{2\kappa} e^{ika} \left[\kappa \cosh(\kappa a) - ik \sinh(\kappa a)\right]$$

$$T = \left|\frac{F}{A}\right|^2 = \left[1 + \frac{V_0^2 \sinh^2(\kappa a)}{4E(V_0 - E)}\right]^{-1}$$

(e) Approximation for $V_0 \gg E$

$$\sinh(\kappa a) \approx \frac{e^{\kappa a}}{2} \implies \sinh^2(\kappa a) \approx \frac{e^{2\kappa a}}{4}$$

$$T \approx \left[1 + \frac{V_0^2 e^{2\kappa a}}{16E(V_0 - E)}\right]^{-1}$$

For $\kappa a \gg 1$:

$$\frac{V_0^2 e^{2\kappa a}}{16E(V_0 - E)} \gg 1 \implies T \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2\kappa a}$$

Let $\eta = \frac{E}{V_0}$:

$$\frac{16E(V_0 - E)}{V_0^2} = 16\eta(1 - \eta)$$

For $V_0 \gg E$ ($\eta \ll 1$), the exponential term dominates:

$$T \sim e^{-2\kappa a}$$

(f) Numerical Calculation for an Electron

Given:

$$\begin{aligned} m_e &= 9.11 \times 10^{-31} \text{ kg}, \\ V_0 &= 5 \text{ eV} = 8.01 \times 10^{-19} \text{ J}, \\ E &= 1 \text{ eV} = 1.60 \times 10^{-19} \text{ J}, \\ a &= 1 \text{ nm} = 10^{-9} \text{ m} \end{aligned}$$

Calculating κ:

$$\kappa \approx 1.14 \times 10^{10} \text{ m}^{-1}$$

Transmission probability:

$$T \approx e^{-22.8} \approx 1.2 \times 10^{-10}$$

(g) Graphical Representation