

100 points total. The following information may or may not be useful

Planck's constant: $\hbar = 1.055 \times 10^{-34}$ J-s = 6.582×10^{-16} eV-s

Speed of light: $c = 3 \times 10^8$ m/s

Mass of the electron: $m_e = 9.1 \times 10^{-31}$ kg

The electron volt: $1 \text{ eV} = 1.6 \times 10^{-19}$ J

$\hbar^2/2m_e = 3.81 \text{ eV-Å}^2$.

1 True/False (18 points)

Circle **T** if the statement is always true. Otherwise circle **F** for false. 2 points each

- ☒ **F** The time-independent Schrödinger equation can be derived from the time-dependent Schrödinger equation.
- ☐ **T** ☒ **F** The uncertainty principle only applies to measurements of position and momentum.
- ☐ **T** ☒ **F** A wave function that is normalized at $t = 0$ will only be normalized at later times if the probability current is zero.
- ☐ **T** ☒ **F** Eigenkets of a Hermitian operator with different eigenvalues are always orthonormal (i.e. orthogonal *and* normalized)
- ☐ **T** ☒ **F** If the Hermitian operator \hat{B} corresponds to a physical property of the quantum-mechanical system, the state function $|\Psi\rangle$ must be an eigenfunction of \hat{B} .
- ☒ **T** ☐ **F** The ground state wavefunction of the one-dimensional simple harmonic oscillator is of the form of a Gaussian, $\psi \propto \exp(-\alpha x^2)$, where α is a constant and x is the displacement of the harmonic oscillator from equilibrium.
- ☐ **T** ☒ **F** When the state function $|\Psi\rangle$ is initially an eigenket of the Hermitian operator \hat{B} with eigenvalue b , and \hat{B} does not commute with the Hamiltonian, we are certain to measure b when the observable corresponding to \hat{B} is measured for all later times.
- ☐ **T** ☒ **F** Linearly independent eigenkets of a Hermitian operator are always orthogonal.
- ☒ **T** ☐ **F** The vibrational motion of an HCl molecule is faster than the rotational motion of an HCl molecule.

2 Multiple Choice (24 points)

Circle **one** answer for each question. 4 points each.

Consider a particle moving in 1 dimension, described at $t = t_0$ by the wave function $\Psi(x, t_0) = A(x)e^{ikx}$, with $A(x)$ real. The probability current evaluated at t_0 is

- a) 0 everywhere.
☒ b) $[\hbar k/m]|\Psi(x, t_0)|^2$
 c) $[\hbar k/(2m)]|\Psi(x, t_0)|^2$
 d) $-\hbar k/m|\Psi(x, t_0)|^2$
 e) none of the above.

$$\begin{aligned}
 J &= \frac{\hbar}{2mi} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) \\
 &= \frac{\hbar}{2mi} \left(ik |\Psi|^2 + ik |\Psi|^2 \right) \\
 &= \frac{\hbar k}{m} |\Psi|^2
 \end{aligned}$$

Consider a quantum bouncing ball, moving in one dimension with the potential $V(y) = mgy$ for $y > 0$ and $V(y) = \infty$ for $y \leq 0$. The solutions to the time-independent Schrödinger equation for this system will have which of the following properties:

- a) They will all be bound states with $\langle p_y \rangle = 0$ and a finite spacing between energy levels.
- b) They will all be free states with a continuous energy spectrum.
- c) There can be bound states and free states.
- d) They must be even or odd functions of y .
- e) a) and d) only.
- f) b) and d) only.
- g) c) and d) only.

Consider a particle, moving in one dimension with the finite square well potential

$$V(x) = \begin{cases} 0, & x < -a \\ -V_0, & -a \leq x \leq a \\ 0, & x > a \end{cases}$$

with V_0 a real positive constant. The solutions to the time-independent Schrödinger equation for this system will have which of the following properties:

- a) They will all be bound states with $\langle p_x \rangle = 0$ and a finite spacing between energy levels.
 - b) They will all be free states with a continuous energy spectrum.
 - c) There can be bound states and free states.
 - d) They must be even or odd functions of x .
 - e) a) and d) only.
 - f) b) and d) only.
 - g) c) and d) only.
- Handwritten note: This was also accepted even though d) is only required for the bound states*

The raising and lowering operators for the simple harmonic oscillator, $\hat{a} = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} + i\hat{p})$ and $\hat{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} - i\hat{p})$, have which of the following properties:

- a) They are Hermitian operators.
- b) They commute with each other.
- c) Given a solution of the harmonic oscillator problem, they can be used to generate new solutions.
- d) all of the above
- e) a) and c) only.
- f) none of the above.

Which of the following would indicate that it may be appropriate to use classical mechanics to treat the motion of a particle?

- a) The particle's de Broglie wavelength is much smaller than length scale over which the particle is confined.
- b) The spacing between energy levels is much smaller than the uncertainty in the particle's energy (e.g. due to thermodynamics).
- c) The particle is moving much slower than the speed of light.
- d) The particle is a simultaneous eigenket of the position and momentum operators such that both can be defined precisely.
- e) The Hamiltonian depends explicitly on time.
- f) a) and c)
- g) b) and c)
- h) a) or b)

When an observable \hat{A} commutes with another observable \hat{B} , it means that

- a) the expectation values $\langle \hat{A} \rangle$ and $\langle \hat{B} \rangle$ are constants of the motion.
- b) one can construct simultaneous eigenkets of \hat{A} and \hat{B} .
- c) the eigenkets of \hat{A} are orthogonal to the eigenkets of \hat{B} .
- d) all of the above.
- e) a) and b) only.
- f) b) and c) only.

3 Operators in Quantum Mechanics (12 points)

Using words and equations, explain what a Hermitian operator is and why Hermitian operators are important in quantum mechanics.

A Hermitian operator satisfies the condition that

$$\langle g | \hat{A} | f \rangle = (\langle f | \hat{A} | g \rangle)^*$$

for any kets $|f\rangle$ and $|g\rangle$. Put another way, the matrix representation is equal to its complex conjugate transpose $A_{ij} = A_{ji}^*$

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{12}^* & A_{22} & \\ A_{13}^* & & \ddots \end{bmatrix}$$

In Bra-ket notation a Hermitian operator can act to the left or the right $\langle g | \hat{A} | f \rangle$

Using the "dagger" notation to denote the Hermitian adjoint \hat{A} Hermitian means $\hat{A}^\dagger = \hat{A}$

Hermitian operators are important in QM b/c they rep. observables.

4 Commuting Observables and Quantum numbers (16 points)

Consider a system with two energy levels, one of which is two-fold degenerate. Take the Hamiltonian \hat{H} for the system to be represented in the orthonormal basis $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$, such that

$$\hat{H}|\alpha\rangle = E_1|\alpha\rangle \quad (4.1)$$

$$\hat{H}|\beta\rangle = E_2|\beta\rangle \quad (4.2)$$

$$\hat{H}|\gamma\rangle = E_2|\gamma\rangle \quad (4.3)$$

In some sense the system is ill defined, in that labeling the states by the energy eigenvalue is ambiguous. If I ask you to describe the E_2 state, you could answer with $|\beta\rangle, |\gamma\rangle$, or in fact any normalized linear combination of the two for an infinite number of possibilities (see part a) below)! This is not a very satisfactory situation. It implies that we need a second quantum number to label the states to remove the ambiguity.

Such a second quantum number can be found using another observable that commutes with the Hamiltonian. For a molecule, this might be a symmetry operator that leaves the molecule unchanged. This problem explores the linear algebra of commuting observables.

a) Show that any linear combination of $|\beta\rangle$ and $|\gamma\rangle$ is also an eigenvector of \hat{H} with eigenvalue E_2 .

b) Write down a matrix representation of \hat{H} in the $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$ basis.

c) Consider the operator \hat{A} such that

$$\hat{A}|\alpha\rangle = a|\alpha\rangle \quad (4.4)$$

$$\hat{A}|\beta\rangle = b|\beta\rangle + ic|\gamma\rangle \quad (4.5)$$

$$\hat{A}|\gamma\rangle = -ic|\beta\rangle + b|\gamma\rangle \quad (4.6)$$

Write down a matrix representation in the $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$ basis and use it to show that \hat{A} commutes with \hat{H} .

d) Using linear combinations of $|\alpha\rangle, |\beta\rangle$, and $|\gamma\rangle$ construct simultaneous eigenkets $|\lambda_H, \lambda_A\rangle$ of \hat{H} and \hat{A} . The labels λ_H and λ_A correspond to the eigenvalues of \hat{H} and \hat{A} , which you need to find as part of this problem.

$$\begin{aligned} 0) \quad \hat{H}(c_1|\beta\rangle + c_2|\gamma\rangle) &= c_1 E_2 |\beta\rangle + c_2 E_2 |\gamma\rangle \\ &= E_2 (c_1|\beta\rangle + c_2|\gamma\rangle) \end{aligned}$$

b)

$$H = \begin{bmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_2 \end{bmatrix}$$

c)

$$\begin{aligned} \langle\alpha|\hat{A}|\alpha\rangle &= a & \langle\alpha|\hat{A}|\beta\rangle &= \langle\alpha|\hat{A}|\gamma\rangle = 0 \\ \langle\beta|\hat{A}|\beta\rangle &= b = \langle\gamma|\hat{A}|\gamma\rangle \\ \langle\beta|\hat{A}|\gamma\rangle &= -ic \end{aligned}$$

$$\Rightarrow A = \begin{bmatrix} a & 0 & 0 \\ 0 & b & -ic \\ 0 & ic & b \end{bmatrix} \quad \text{Hermitian } \checkmark$$

$$\begin{bmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_2 \end{bmatrix}$$

$$AH = \begin{bmatrix} a & 0 & 0 \\ 0 & b & -ic \\ 0 & ic & b \end{bmatrix} \begin{bmatrix} aE_1 & 0 & 0 \\ 0 & E_2 & -icE_2 \\ 0 & icE_2 & E_2b \end{bmatrix}$$

$$\begin{bmatrix} a & 0 & 0 \\ 0 & b & -ic \\ 0 & ic & b \end{bmatrix}$$

$$HA = \begin{bmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_2 \end{bmatrix} \begin{bmatrix} aE_1 & 0 & 0 \\ 0 & bE_2 & -icE_2 \\ 0 & icE_2 & bE_2 \end{bmatrix}$$

$$HA = AH \Rightarrow [H, A] = 0$$

Eigenvalues

$$\lambda_A = a \Rightarrow X = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \Rightarrow |E_1, a\rangle = |x\rangle$$

For other two, work in orthogonal subspace

$$(b \mp ic) \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} ic & b \\ b & -ic \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

$$\tilde{\lambda}_F = \frac{1}{\sqrt{2}} \begin{bmatrix} \tilde{F} \\ 1 \\ 0 \end{bmatrix}$$

$$|E_2, b+ic\rangle = \frac{1}{\sqrt{2}} |\beta\rangle + \frac{i}{\sqrt{2}} |\alpha\rangle$$

$$|E_2, b-ic\rangle = \frac{1}{\sqrt{2}} |\beta\rangle - \frac{i}{\sqrt{2}} |\alpha\rangle$$

$$(a-\lambda_A)(b-\lambda_A)^2 - c^2 = 0$$

$$\det \begin{pmatrix} a-\lambda_A & 0 & 0 \\ 0 & b-\lambda_A & -ic \\ 0 & ic & b-\lambda_A \end{pmatrix} = 0$$

\Rightarrow

$$\lambda_A = a$$

$$\lambda_A = b+ic$$

$$\lambda_A = b-ic$$

3 eigenvalues

5 Particle on a Ring (15 points)

Consider a particle of mass m confined to one dimensional motion with $V = 0$ and periodic boundary conditions such that

$$\psi(x+L) = \psi(x)$$

This could, for example, represent the motion of a particle confined to motion on a thin ring with radius R , circumference $L = 2\pi R$, and position measured along the ring $x = R\theta$. You can see then that the wave function must be periodic with respect to going around the ring. If I go around once and come back to where I started, I should have the same value for the wave function.

Solve the time-independent Schrödinger equation ($\hat{H}\psi(x) = E\psi(x)$) for this system and find the stationary states and energy eigenvalues. Are the energy levels degenerate? If so, what is the degeneracy of each energy level (i.e. how many linearly independent eigenfunctions share the same energy)?

The TISE reads
$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{w/ } k = \sqrt{\frac{2mE}{\hbar^2}}$$

\Rightarrow solutions are oscillatory $\sin kx$ and $\cos kx$ or e^{ikx} and e^{-ikx}

Use $\{e^{ikx} \text{ and } e^{-ikx}\}$ must have $e^{ikx} = e^{ik(x+L)}$

Energy the same \Rightarrow 2-fold degenerate.
(doesn't matter which direction around the ring you go)

$$\Rightarrow e^{ikL} = 1$$

Normalization $\int_0^L |\psi|^2 dx = 1$

$$\Rightarrow \psi_{\pm} = \frac{1}{\sqrt{L}} e^{\pm ikx}$$

$$\begin{aligned} \Rightarrow k &= n \frac{2\pi}{L} \\ \text{w/ } n &= 1, 2, 3, \dots \\ E &= \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2mL^2} n^2 \\ &= \frac{\hbar^2}{8m\pi^2 R^2} n^2 \\ &= \frac{\hbar^2}{2mR^2} n^2 \end{aligned}$$

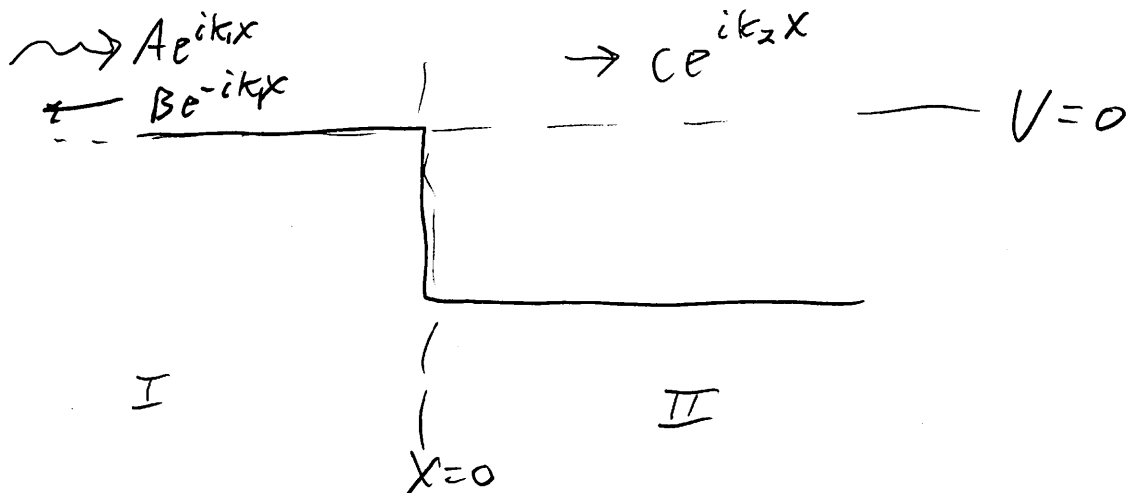
Note that any linear combination of ψ_{\pm} will also work, since 2-fold degenerate. e.g. \sin and \cos

6 Scattering from a "Cliff" (15 points)

Consider a particle with energy $E = V_0/3$ incident from the left on a potential with an abrupt drop.

$$V(x) = \begin{cases} 0, & x < 0 \\ -V_0, & x \geq 0 \end{cases}$$

with V_0 a real positive constant. Calculate the probability that the particle is reflected from the abrupt drop.



Region I:

$$\psi_I = A e^{ik_1 x} + B e^{-ik_1 x}$$

$$k_1 = \sqrt{\frac{2m(V_0/3)}{\hbar^2}}$$

Region II

$$\psi_{II} = C e^{ik_2 x}$$

$$k_2 = \sqrt{\frac{2m(4V_0/3)}{\hbar^2}}$$

$$k_2 = 2k_1$$

B.C.'s

$$\psi_I(0) = \psi_{II}(0) \Rightarrow A + B = C$$

$$\psi'_I(0) = \psi'_{II}(0) \Rightarrow ik_1 A - ik_1 B = 2ik_1 C$$

$$A - B = 2C$$

$$R = \frac{J_{ref}}{J_{in}} = \frac{\frac{\hbar k_1}{m} |B|^2}{\frac{\hbar k_1}{m} |A|^2} = \frac{1}{9} = R$$

$$2A = 3C \Rightarrow C = \frac{2}{3} A$$

$$\Rightarrow B = -\frac{1}{3} A$$

Even More Space! (If you would like to be graded on this work, please indicate which problem corresponds to which work)