SECOND PUBLIC EXAMINATION

Honour School of Physics Part A: 3 and 4 Year Courses

Honour School of Physics and Philosophy Part A

A3: QUANTUM PHYSICS

TRINITY TERM 2022

Friday, 17 June, 2.30 pm - 5.30 pm

Answer all of Section A and three questions from Section B.

For Section A start the answer to each question on a fresh page. For Section B start the answer to each question in a fresh book.

A list of physical constants and conversion factors accompanies this paper.

The numbers in the margin indicate the weight that the Examiners expect to assign to each part of the question.

Do NOT turn over until told that you may do so.

Section A

1. (a) Considering the operator $\hat{\pi} = -i\hbar \frac{\partial}{\partial x} + f(x)$, where f(x) is an integrable function of x, find the commutators $[\hat{x}, \hat{\pi}]$ and $[\hat{x}, \hat{\pi}^2]$.

(b) Find an eigenfunction $\phi(x)$ for the operator $\hat{\pi}$ with eigenvalue $\hbar k$. Determine if it satisfies the eigenvalue equation for the energy of a free particle,

$$\frac{\hat{\pi}^2}{2m}\phi(x) = \frac{(\hbar k)^2}{2m}\phi(x).$$
[4]

2. (a) Derive Ehrenfest's theorem for $d\langle x \rangle/dt$, where $\langle x \rangle$ is the expectation value of the operator \hat{x} . Show that the quantum analogue to Newton's second law is $\langle F \rangle = d\langle p \rangle/dt$, where F is the negative differential change in a static potential energy with respect to position x.

(b) For a potential $V(x) = kx^2$, show that $\langle F \rangle$ corresponds to the classical equation with the replacement $x \to \langle x \rangle$. Does the same hold for the potential $V(x) = \lambda x^3$? If not, discuss whether the magnitude of $d\langle p \rangle/dt$ would be larger or smaller than the classical analogue in this case.

3. (a) Individual unpolarised spin-1/2 particles with momentum p are released in the direction of a barrier. A slit of width similar to the particle wavelength is cut into the barrier. Sketch the intensity distribution of the particles on a screen placed far behind the barrier. A second slit of equal width is cut into the barrier near to the first. Sketch the resulting intensity distribution.

(b) A Stern-Gerlach filter that passes particles with spin $+\hbar/2$ in the z direction is placed in front of one of the slits. Describe qualitatively the intensity distribution on the screen for the following cases:

(i) the particles are sent directly to the slits;

(ii) before approaching the slits the particles go through a filter passing spin $+\hbar/2$ particles in the z direction;

(iii) before approaching the slits the particles go through a filter passing spin $+\hbar/2$ particles in the x direction.

Compare the relative amplitudes of the central peak between the three cases.

4. (a) An electron in a hydrogen atom is in the n = 2, l = 1 state. Sketch its radial wavefunction $R_{21}(r)$. The electron radiates a photon to go to the n = 1, l = 0 state. Sketch the resulting radial wavefunction $R_{10}(r)$. Express the probability of finding the n = 1 electron at a radius r in terms of this wavefunction. Sketch this probability as a function of r.

(b) Express the matrix element describing the electron's transition from the initial state to the final state in terms of $R_{21}(r)$ and $R_{10}(r)$ (you do not need to determine the explicit form of these functions). You may wish to use $Y_0^0 = \frac{1}{2\sqrt{\pi}}$ and $Y_1^0 = \frac{\sqrt{3}}{2\sqrt{\pi}} \cos \theta$. [3]

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5. (a) State the quantum numbers of the hydrogen energy levels and give their physical interpretation. Express the energy levels E_n in terms of the fine structure constant α and other quantities, and derive their degeneracy (including spin).

[The Rydberg energy can be expressed as $E_{R,\infty} = m_e c^2 \alpha^2 / 2.$]

(b) A correction to these energy levels results from the interaction of the electron spin with the magnetic field arising from the electron's motion through the electric field produced by the proton. The potential describing this interaction is

$$V = \frac{\alpha \hbar \vec{L} \cdot \vec{S}}{2\mu^2 c r^3}.$$

Use first-order perturbation theory to find the energy correction ΔE , and determine the ratio $\Delta E/E_n$. You may wish to use a basis of eigenstates for $\vec{J}^2 = (\vec{L} + \vec{S})^2$ and \vec{L}^2 , and note that the electron has spin 1/2.

[In this basis

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{n^3 a_0^3 l(l+1/2)(l+1)},$$

where $a_0 = \hbar/(\alpha \mu c)$.]

Section B

6. Consider a harmonic oscillator with Hamiltonian $\hat{H} = \hat{p}^2/2m + m\omega^2 \hat{x}^2/2$.

(a) Classically, the oscillator's position can be expressed as $x(t) = A \sin(\omega t + \phi)$, where A is an amplitude and ϕ is a phase. If at time t = 0 the phase is unknown, the mean of the possible positions is $\overline{x} = \frac{1}{2\pi} \int_0^{2\pi} x(0) \, \mathrm{d}\phi$.

(i) Find \overline{x} and the means $\overline{x^2}$, \overline{p} , and $\overline{p^2}$, using the classical expression for position.

(ii) Write the above means in terms of the energy $E = A^2 m \omega^2/2$, and find the position and momentum variances $\Delta x^2 = \overline{x^2} - \overline{x}^2$ and $\Delta p^2 = \overline{p^2} - \overline{p}^2$.

(b) Defining the quantum operator $\hat{a} = (m\omega/2\hbar)^{1/2}\hat{x} + i\hat{p}/(2m\hbar\omega)^{1/2}$, find $[\hat{a}, \hat{a}^{\dagger}]$ and write the Hamiltonian in terms of \hat{a} and \hat{a}^{\dagger} . [4]

(c) Given that the state $|n\rangle$ satisfies the eigenvalue equation $\hat{a}^{\dagger}\hat{a}|n\rangle = n|n\rangle$, where n is an integer, find $\hat{a}|n\rangle$ and $\hat{a}^{\dagger}|n\rangle$. Determine the ground-state wave function $\langle x|0\rangle$ up to the normalization factor N.

(d) For a given state $|n\rangle$ find $\langle x\rangle$, $\langle x^2\rangle$, $\langle p\rangle$, $\langle p^2\rangle$. Use these to evaluate Δx^2 , Δp^2 , and $\Delta x \Delta p$. Compare the latter to $\Delta x \Delta p$ determined using the classical means in part (a).

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7. Consider the quantum-mechanical description of a particle of mass M confined to a cylindrical box with radius a and length L. In cylindrical coordinates (r, ϕ, z) the free-particle Hamiltonian is

$$\hat{H} = \frac{1}{2M} \left(\hat{p}_r^2 + \hat{p}_z^2 + \frac{\hat{L}_z^2}{r^2} \right),$$

where \hat{p}_z is the momentum operator in the z direction, \hat{L}_z is the angular momentum operator in the z direction, and \hat{p}_r^2 acts on a radial wavefunction as follows:

$$\langle r|\hat{p}_{r}^{2}|\psi\rangle = -\hbar^{2}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)\langle r|\psi\rangle.$$

(a) If the particle is confined to the walls at r = a, write down the Schrödinger equation for the energy eigenstates $\psi_{n,m}(\phi, z)$. Provide a general solution using coordinates where the box is centred at z = 0, including relevant normalization factors. Define the quantum numbers n and m, state their possible values and give an expression for the energy eigenvalues. Find the energies of the two lowest energy states when L = a. Sketch the real part of the wavefunctions of these two states, on separate graphs, as a function of ϕ and as a function of z (so four graphs in all).

(b) If the particle can move freely inside the cylindrical box but cannot escape, write the wavefunction as $\Psi(\vec{r}) = \psi_{n,m}(\phi, z)R(r)$ and use the Schrödinger equation to derive an equation for R(r). In the ground state, $R(r) \approx 1 - (kr)^2/4 + (kr)^4/64$ for $r \leq a$. Use the boundary condition at r = a to find k for this ground state. Show that this state satisfies the Schrödinger equation if one neglects a term of order $C(kr)^4$, where C is a constant. Neglecting this term, determine the energy of the ground state in terms of a and L.

8. A particle is in a one-dimensional box with impenetrable walls at $x = \pm a$.

(a) Give expressions for the normalized wavefunction and energy of the particle in terms of the energy quantum number n and mass m.

(b) An infinitesimally thin wall at x = 0 is adiabatically introduced into the system. Taking the wall to be impenetrable once it is fully introduced, find the new normalized wavefunction and energy if the particle is initially in the (i) ground or (ii) first excited state. Infer the energy required to insert the barrier for each energy state.

(c) If the impenetrable wall is adiabatically introduced near the edge of the box, $x = a - \delta$ where $\delta < a$, sketch the resulting wavefunction for a particle initially in the ground state.

(d) Consider the case of a penetrable thin wall introduced suddenly at $x = a - \delta$. If the particle is initially in the ground state, determine the probability of observing the particle in the region $a - \delta < x < a$ immediately after insertion, to lowest order in $\epsilon \equiv \frac{\delta}{2a}$. Compare the result to the classical probability. Sketch the wavefunction of the new ground state.

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9. Double-well potentials are common in nature. For example, the ammonia molecule is composed of three hydrogen atoms in a plane with a nitrogen atom on one side of the plane. Defining x to be the nitrogen position relative to the plane, the potential experienced by the nitrogen atom can be approximated by infinite walls at $x = \pm \frac{a}{2}$, a potential barrier of height V_0 in the middle $(-b \le x \le b)$, and zero potential in between $(-\frac{a}{2} \le x < -b \text{ and } b < x \le \frac{a}{2})$.

(a) The wavefunction can be expressed as $\Psi(x) = A\psi(x)$ in each region of constant potential, where A is the normalization factor in that region. Considering solutions with $0 < E < V_0$, use the symmetry of the potential and the constraints at the boundaries $x = -\frac{a}{2}$ and $x = \frac{a}{2}$ to find ground-state expressions for $\psi(x)$ for $-\frac{a}{2} \leq x < -b$, $-b \leq x \leq b$ and $b < x \leq \frac{a}{2}$.

(b) Again use the symmetry and boundary conditions to find expressions for $\psi(x)$ for the first excited state. Sketch the wavefunctions for the ground state and the first excited state and use the boundary conditions at x = -b to find the transcendental equations determining the bound states. Discuss how the energy changes as (i) b and (ii) V_0 are increased.

(c) Consider ammonia with the nitrogen atom prepared at t = 0 in the state $|\Psi\rangle = \sqrt{\frac{1}{2}} (|\Psi_1\rangle + |\Psi_2\rangle)$, where $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are the eigenfunctions for the ground and first excited energy levels E_1 and E_2 respectively. Sketch the wavefunction $\langle x|\Psi\rangle$ and obtain the probability of finding the system in this same state at a time t. Give a physical description of the time dependence.

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A3: Quantum Mechanics and Further Quantum Mechanics Final Paper 2023

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0	Р	\mathbf{E}	\mathbf{R}	А
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A Section A

A.1 1

A.1.a (a)

We want to find the commutators $[\hat{x},\hat{\pi}]$ and $\big[\hat{x},\hat{\pi}^2\big].$

For the first commutator, $[\hat{x}, \hat{\pi}] = \hat{x}\hat{\pi} - \hat{\pi}\hat{x}$. Applying the definition of $\hat{\pi}$, we get:

$$[\hat{x},\hat{\pi}] = \hat{x} \left(-i\hbar \frac{\partial}{\partial x} + f(x) \right) - \left(-i\hbar \frac{\partial}{\partial x} + f(x) \right) \hat{x}$$
(A.1.a.1)

$$= -i\hbar x \frac{\partial}{\partial x} + x f(x) + i\hbar \frac{\partial}{\partial x} x - f(x)x$$
(A.1.a.2)

(A.1.a.3)

We can rearrange the terms and use the product rule to find the derivative of x with respect to x:

$$[\hat{x},\hat{\pi}] = -i\hbar x \frac{\partial}{\partial x} + xf(x) + i\hbar \left(\frac{\partial x}{\partial x} + x\frac{\partial}{\partial x}\right) - f(x)x \qquad (A.1.a.4)$$

$$= -i\hbar x \frac{\partial}{\partial x} + xf(x) + i\hbar(1 + x\frac{\partial}{\partial x}) - f(x)x$$
(A.1.a.5)

Now, we can combine the terms:

$$[\hat{x},\hat{\pi}] = -i\hbar x \frac{\partial}{\partial x} + xf(x) + i\hbar + i\hbar x \frac{\partial}{\partial x} - f(x)x$$
(A.1.a.7)

$$=i\hbar.$$
 (A.1.a.8)

For the second commutator, $[\hat{x}, \hat{\pi}^2] = \hat{x}\hat{\pi}^2 - \hat{\pi}^2\hat{x}$, we have:

$$\left[\hat{x}, \hat{\pi}^2\right] = \hat{x} \left(-i\hbar \frac{\partial}{\partial x} + f(x)\right)^2 - \left(-i\hbar \frac{\partial}{\partial x} + f(x)\right)^2 \hat{x}$$
(A.1.a.9)

$$= \hat{x} (\hat{\pi}\hat{\pi}) - (\hat{\pi}\hat{\pi}) \hat{x}$$
(A.1.a.10)
= $[\hat{x}, \hat{\pi}\hat{\pi}]$ (A.1.a.11)

$$= [\hat{x}, \hat{\pi}] \hat{\pi} + \hat{\pi} [\hat{x}, \hat{\pi}]$$
(A.1.a.12)
(A.1.a.12)

$$=i\hbar\hat{\pi}+\hat{\pi}i\hbar \tag{A.1.a.13}$$

$$=2i\hbar\hat{\pi}.$$
 (A.1.a.14)

A.1.b (b)

We have the eigenfunction $\phi(x)$ as:

$$\phi(x) = C e^{ikx - i\int \frac{f(x)}{\hbar} dx}$$

Now we need to check if this eigenfunction satisfies the eigenvalue equation for the energy of a free particle:

$$\frac{\hat{\pi}^2}{2m}\phi(x) = \frac{(\hbar k)^2}{2m}\phi(x)$$
 (A.1.b.1)

Applying the operator $\frac{\hat{\pi}^2}{2m}$ on $\phi(x)$:

$$\frac{\hat{\pi}^2}{2m}\phi(x) = \frac{1}{2m}(-i\hbar\frac{\partial}{\partial x} + f(x))^2\phi(x)$$
(A.1.b.2)

$$=\frac{1}{2m}(-i\hbar\frac{\partial}{\partial x}+f(x))(-i\hbar\frac{\partial}{\partial x}+f(x))Ce^{ikx-i\int\frac{f(x)}{\hbar}\,dx}\qquad(A.1.b.3)$$

Since the expression is quite complex, let's apply the operator step by step. First, let's apply $(-i\hbar\frac{\partial}{\partial x} + f(x))$ on $\phi(x)$:

$$(-i\hbar\frac{\partial}{\partial x} + f(x))\phi(x)$$
 (A.1.b.4)

$$= -i\hbar \frac{\partial}{\partial x} C e^{ikx - i\int \frac{f(x)}{\hbar} dx} + f(x) C e^{ikx - i\int \frac{f(x)}{\hbar} dx}$$
(A.1.b.5)

$$= -i\hbar C\left(ik + \frac{f(x)}{\hbar}\right)e^{ikx - i\int\frac{f(x)}{\hbar}\,dx} + f(x)Ce^{ikx - i\int\frac{f(x)}{\hbar}\,dx}$$
(A.1.b.6)

$$=\hbar kCe^{ikx-i\int\frac{f(x)}{\hbar}\,dx}\tag{A.1.b.7}$$

Now, let's apply the operator $(-i\hbar\frac{\partial}{\partial x}+f(x))$ on the resulting expression:

$$(-i\hbar\frac{\partial}{\partial x} + f(x))\hbar kCe^{ikx - i\int\frac{f(x)}{\hbar}dx}$$
(A.1.b.8)

$$= -i\hbar \frac{\partial}{\partial x} (\hbar k C e^{ikx - i\int \frac{f(x)}{\hbar} dx}) + f(x)\hbar k C e^{ikx - i\int \frac{f(x)}{\hbar} dx}$$
(A.1.b.9)

$$= -i\hbar\hbar k^2 C e^{ikx-i\int \frac{f(x)}{\hbar} dx} + f(x)\hbar k C e^{ikx-i\int \frac{f(x)}{\hbar} dx}$$
(A.1.b.10)

$$=\hbar^2 k^2 C e^{ikx-i\int \frac{f(x)}{\hbar} dx} \tag{A.1.b.11}$$

Now we have:

$$\frac{\hat{\pi}^2}{2m}\phi(x) = \frac{\hbar^2 k^2 C e^{ikx - i\int \frac{f(x)}{\hbar} \, dx}}{2m}$$
(A.1.b.12)

Now let's compare this result with the right-hand side of the eigenvalue equation for the energy of a free particle:

$$\frac{(\hbar k)^2}{2m}\phi(x) = \frac{\hbar^2 k^2}{2m} C e^{ikx - i\int \frac{f(x)}{\hbar} dx}$$
(A.1.b.13)

Comparing both expressions, we see that they are equal:

$$\frac{\hat{\pi}^2}{2m}\phi(x) = \frac{(\hbar k)^2}{2m}\phi(x)$$
 (A.1.b.14)

Thus, the given eigenfunction $\phi(x)$ does satisfy the eigenvalue equation for the energy of a free particle.

A.2 2

A.2.a (a)

To derive Ehrenfest's theorem for $\frac{d\,\langle x\rangle}{d\,t},$ we start with the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$
 (A.2.a.1)

We'll also consider the complex conjugate of the Schrödinger equation:

$$-i\hbar\frac{\partial}{\partial t}\left\langle\psi(t)\right\rangle = \left\langle\psi(t)\right|\hat{H}$$
(A.2.a.2)

Now, we want to compute $\frac{d\langle x\rangle}{dt}$, so we'll take the derivative of the expectation value of the operator \hat{x} with respect to time:

$$\frac{d\langle x\rangle}{dt} = \frac{d}{dt}t\langle\psi(t)|\hat{x}|\psi(t)\rangle \tag{A.2.a.3}$$

$$= \frac{\partial}{\partial t} \langle \psi(t) | \hat{x} | \psi(t) \rangle + \langle \psi(t) | \hat{x} \frac{\partial}{\partial t} | \psi(t) \rangle$$
(A.2.a.4)

Using the Schrödinger equation and its complex conjugate, we replace the time derivatives of the wave function and its conjugate:

$$\frac{d\langle x\rangle}{dt} = \frac{1}{i\hbar} \langle \psi(t) | \hat{H}\hat{x} | \psi(t) \rangle - \frac{1}{i\hbar} \langle \psi(t) | \hat{x}\hat{H} | \psi(t) \rangle$$
(A.2.a.5)

$$= \frac{1}{i\hbar} \langle \psi(t) | [\hat{H}, \hat{x}] | \psi(t) \rangle$$
(A.2.a.6)

Since $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, we have:

$$\frac{d\langle x\rangle}{dt} = \frac{1}{i\hbar} \langle \psi(t) | \left[\frac{\hat{p}^2}{2m} + V(x), \hat{x} \right] | \psi(t) \rangle$$
(A.2.a.7)

$$= \frac{1}{i\hbar} \langle \psi(t) | \left[\frac{\hat{p}^2}{2m}, \hat{x} \right] | \psi(t) \rangle + \frac{1}{i\hbar} \langle \psi(t) | \left[V(x), \hat{x} \right] | \psi(t) \rangle$$
(A.2.a.8)

Since V(x) is a function of \hat{x} , $[V(x), \hat{x}] = 0$, and we only need to compute the commutator $[\frac{\hat{p}^2}{2m}, \hat{x}]$. Using the fact that $[\hat{p}, \hat{x}] = -i\hbar$, we have:

$$\left[\frac{\hat{p}^2}{2m}, \hat{x}\right] = \frac{1}{2m} (\hat{p}(\hat{p}\hat{x} + \hat{x}\hat{p}) - (\hat{x}\hat{p} + \hat{p}\hat{x})\hat{p})$$
(A.2.a.9)

$$= \frac{1}{2m} (\hat{p}\hat{p}\hat{x} + \hat{p}\hat{x}\hat{p} - \hat{x}\hat{p}\hat{p} - \hat{p}\hat{x}\hat{p})$$
(A.2.a.10)

$$=\frac{1}{2m}(\hat{p}\hat{p}\hat{x}-\hat{x}\hat{p}\hat{p}) \tag{A.2.a.11}$$

$$= \frac{1}{2m} [\hat{p}, \hat{p}] \hat{x}$$
 (A.2.a.12)

$$= 0$$
 (A.2.a.13)

Therefore, we have

$$\frac{d\langle x\rangle}{dt} = \frac{1}{m}\langle p\rangle \tag{A.2.a.14}$$

which is Ehrenfest's theorem for $\frac{d\langle x\rangle}{dt}$. To show that the quantum analogue to Newton's second law is $\langle F \rangle = \frac{d\langle p \rangle}{dt}$, we need to compute $\frac{d\langle p \rangle}{dt}$ and compare it to the expectation value of the force. We'll follow a similar procedure as above:

$$\frac{d \langle p \rangle}{dt} \tag{A.2.a.15}$$

$$= \frac{1}{i\hbar} \langle \psi(t) | \left[\hat{H}, \hat{p} \right] | \psi(t) \rangle \tag{A.2.a.16}$$

We compute the commutator $[\hat{H}, \hat{p}]$:

$$[\hat{H}, \hat{p}] = \left[\frac{\hat{p}^2}{2m} + V(x), \hat{p}\right]$$
(A.2.a.17)

$$= \left[\frac{\hat{p}^2}{2m}, \hat{p}\right] + \left[V(x), \hat{p}\right]$$
(A.2.a.18)

Since $\frac{\hat{p}^2}{2m}$ is a function of \hat{p} , $[\frac{\hat{p}^2}{2m}, \hat{p}] = 0$. We only need to compute the commutator $[V(x), \hat{p}]$. Using the fact that $[\hat{x}, \hat{p}] = i\hbar$, we have:

$$[V(x),\hat{p}] = (\partial_x V(x))[\hat{x},\hat{p}]$$
(A.2.a.19)

$$= -i\hbar(\partial_x V(x)) \tag{A.2.a.20}$$

Now, substituting this back into our expression for $\frac{d \langle p \rangle}{dt}$:

$$\frac{d \langle p \rangle}{dt} = \frac{1}{i\hbar} \langle \psi(t) | \left(-i\hbar(\partial_x V(x)) \right) | \psi(t) \rangle$$
 (A.2.a.21)

$$= -\langle \psi(t) | (\partial_x V(x)) | \psi(t) \rangle$$
 (A.2.a.22)

$$= -\langle F \rangle$$
 (A.2.a.23)

This demonstrates that the quantum analogue to Newton's second law is $\langle F \rangle = \frac{d \langle p \rangle}{dt}$, where F is the negative differential change in a static potential energy with respect to position x.

A.2.b (b)

For the potential $V(x) = kx^2$, we have:

$$\langle F \rangle = -\frac{d \langle V \rangle}{dx}$$
 (A.2.b.1)

$$= -\frac{d}{dx} \left(\int \psi(x) V(x) \psi(x) dx \right)$$
(A.2.b.2)

$$= -\int \psi(x) \frac{dV(x)}{dx} \psi(x) dx \qquad (A.2.b.3)$$

$$= -\int \psi^{(x)}(2kx)\psi(x)\mathrm{d}x \qquad (A.2.b.4)$$

$$= -2k \int x |\psi(x)|^2 \mathrm{d}x \tag{A.2.b.5}$$

$$= -2k \langle x \rangle \tag{A.2.b.6}$$

This equation is the same as the classical equation of motion with the replacement $x \to \langle x \rangle$.

For the potential $V(x) = \lambda x^3$, we have:

$$\langle F \rangle = -\frac{d \langle V \rangle}{dx} \tag{A.2.b.7}$$

$$= -\frac{d}{dx} \left(\int \psi(x) V(x) \psi(x) dx \right)$$
(A.2.b.8)

$$= -\int \psi(x) \frac{dV(x)}{dx} \psi(x) dx \qquad (A.2.b.9)$$

$$= -\int \psi^{(x)}(3\lambda x^2)\psi(x)\mathrm{d}x \qquad (A.2.b.10)$$

$$= -3\lambda \int x^2 |\psi(x)|^2 \mathrm{d}x \qquad (A.2.b.11)$$

$$\frac{d\langle p\rangle}{dt} = \frac{1}{i\hbar} \langle \psi(t) | \left(-i\hbar(\partial_x V(x)) \right) | \psi(t) \rangle$$
(A.2.b.12)

$$= \frac{1}{i\hbar} \langle \psi(t) | (-i\hbar(3\lambda x^2)) | \psi(t) \rangle$$
 (A.2.b.13)

$$= -3\lambda \langle \psi(t) | x^2 | \psi(t) \rangle \tag{A.2.b.14}$$

Here we see that $\langle F \rangle$ and $\frac{d \langle p \rangle}{dt}$ are not proportional, meaning the quantum result does not correspond to the classical result with a simple replacement. The magnitude of $\frac{d \langle p \rangle}{dt}$ is larger than the classical analogue.

A.3 3

A.3.a (a)

In the single slit experiment, the wave nature of the particles causes them to diffract as they pass through the slit, resulting in an intensity distribution pattern on the screen that has a central maximum and several smaller maxima on either side. This is the diffraction pattern. In the double slit experiment, the particles pass through both slits and their waves interfere with each other, resulting in an interference pattern on the screen. This pattern consists of maxima and minima of intensity caused by the constructive and destructive interference of the waves. The interference pattern of the double slit experiment is modulated by the diffraction pattern of the single slit experiment. This means that the peaks of the interference pattern align with the envelope of the diffraction pattern, and the intensity of the interference pattern never exceeds the intensity of the diffraction pattern at any given point. The Intensity for single slit diffraction pattern will be given by sinc x which can be simplified to $\frac{\sin x}{x}$ and when we can let w be the width of each slit x be the horizontal breadth of the screen and L be the distance to the screen

$$I(x) = I_0 \operatorname{sinc}^2 \left(\frac{\pi x w}{\lambda L}\right) \tag{A.3.a.1}$$

Recall that sinc 0 = 1 So then we can modulate this by $\cos^2 x$ to get the effect of the double slit.



Figure 1: Double and single slit

A.3.b (b)

(i) When the particles are sent directly to the slits, the Stern-Gerlach filter in front of one of the slits will only allow particles with spin $+\frac{\hbar}{2}$ in the z direction

to pass. This will result in an uneven distribution of particles on the screen, with a lower intensity on the side corresponding to the filtered slit. The central peak's amplitude will be less than in a standard double-slit experiment due to the reduced number of particles contributing to the interference at this point.

(ii) If the particles are first passed through a filter that only allows spin $+\frac{\hbar}{2}$ in the z direction, all particles reaching the double-slit setup will have this specific spin orientation. The Stern-Gerlach filter in front of one of the slits will not affect these particles, leading to a standard double-slit interference pattern on the screen. The amplitude of the central peak will be the same as in a standard double-slit experiment, as all particles contribute to the interference at this point.

(iii) If the particles first pass through a filter that only allows particles with $\sinh + \frac{\hbar}{2}$ in the x direction, the Stern-Gerlach filter in front of one of the slits will cause a change in the spin orientation of the particles to the z direction. This change in spin orientation will not preferentially block or allow any particles, leading to a standard double-slit interference pattern on the screen. However, the central peak's amplitude will be less than in case (ii) due to the change in spin orientation caused by the Stern-Gerlach filter.

The relative amplitudes will therefore be (ii) > (iii) > (i)

A.4 4 A.4.a (a)



Figure 2: radial wavefunction $R_{21}(r)$



Figure 3: radial wavefunction $R_{10}(r)$



Figure 4: Probability Density

A.4.b (b)

Lets assume that the radial wavefunctions $R_{10}(r)$ and $R_{21}(r)$ are normalized. The matrix element describing the electron's transition from the initial state to the final state is given by:

$$\langle 1, 0|r|2, 1\rangle = \int_0^\infty r^2 R_{10}(r) R_{21}(r) dr \int_0^{2\pi} \int_0^\pi Y_0^{0*}(\theta, \phi) Y_1^0(\theta, \phi) \sin \theta d\theta d\phi.$$
(A.4.b.1)

This integral represents the overlap of the final state wavefunction $R_{10}(r)$ and the initial state wavefunction $R_{21}(r)$, weighted by the spherical harmonics Y_0^0 and Y_1^0 , which describe the angular part of the transition.

The integral over the angular part can be simplified using the orthogonality of the spherical harmonics, but the radial part cannot be simplified without the explicit forms of the radial wavefunctions $R_{10}(r)$ and $R_{21}(r)$.

The probability of finding the electron in the n = 1 state at a radius r is given by:

$$P(r) = 4\pi r^2 |R_{10}(r)|^2.$$
(A.4.b.2)

This expression represents the probability density of finding the electron at a radius r in the n = 1 state. The factor of $4\pi r^2$ comes from the volume element in spherical coordinates.

A.5 5

A.5.a (a)

The quantum numbers for hydrogen energy levels are

$$n = 1, 2, 3, \dots$$
 (principal quantum number) (A.5.a.1)

$$l = 0, 1, 2, \dots, n-1$$
 (azimuthal quantum number) (A.5.a.2)

$$m_l = -l, -l+1, \dots, l-1, l$$
 (magnetic quantum number) (A.5.a.3)

$$m_s = \pm \frac{1}{2}$$
 (spin quantum number) (A.5.a.4)

(A.5.a.5)

The energy levels of the hydrogen atom can be expressed in terms of the fine structure constant α , the electron mass m_e , the speed of light c, and the principal quantum number n as follows:

$$E_n = -\frac{m_e c^2 \alpha^2}{2n^2} \tag{A.5.a.6}$$

The degeneracy of these energy levels, including spin, is given by the number of states with the same energy. This is equal to the number of possible combinations of the quantum numbers, which is $2n^2$. The factor of 2 comes from the two possible values of the spin quantum number.

$$g_n = 2\sum_{l=0}^{n-1} (2l+1) = 2n^2$$
(A.5.a.7)

The degeneracy g_n accounts for the number of possible states for a given energy level n, including the electron's spin.

A.5.b (b)

The potential describing the interaction of the electron spin with the magnetic field arising from the electron's motion through the electric field produced by the proton is given by:

$$V = \frac{\alpha \hbar \vec{L} \cdot \vec{S}}{2\mu^2 cr^3} \tag{A.5.b.1}$$

We can use first-order perturbation theory to find the energy correction ΔE . The first-order correction to the energy is given by the expectation value of the perturbation:

$$\Delta E = \langle \psi | V | \psi \rangle \tag{A.5.b.2}$$

where ψ is the wavefunction of the state. In this case, we can use a basis of eigenstates for $\vec{J}^2 = (\vec{L} + \vec{S})^2$ and \vec{L}^2 , and note that the electron has spin 1/2. Using the given expectation value for $1/r^3$, we find:

$$\Delta E = \frac{\alpha \hbar \langle \psi | \vec{L} \cdot \vec{S} | \psi \rangle}{2\mu^2 c n^3 a_0^3 l (l+1/2) (l+1)}$$
(A.5.b.3)

The ratio $\Delta E/E_n$ is then given by:

$$\frac{\Delta E}{E_n} = \frac{\alpha \hbar \langle \psi | \vec{L} \cdot \vec{S} | \psi \rangle}{2\mu^2 c n^3 a_0^3 l (l+1/2) (l+1) E_n}$$
(A.5.b.4)

Substituting the given values into the above equation, we find:

$$\frac{\Delta E}{E_n} = -\frac{137}{6r^3} \tag{A.5.b.5}$$

B Section **B**

B.6 6

B.6.a (a)

 At

$$x(t) = A\sin(\omega t + \phi) \tag{B.6.a.1}$$

time
$$t = 0$$
: (B.6.a.2)

$$x(0) = A\sin(\phi) \tag{B.6.a.3}$$

Now, we find the mean position:

$$\bar{x} = \frac{1}{2\pi} \int_0^{2\pi} A \sin(\phi) d\phi$$
 (B.6.a.5)
 $\bar{x} = 0$ (B.6.a.6)

Similarly, we find other means:

$$\bar{x^2} = \frac{1}{2\pi} \int_0^{2\pi} A^2 \sin^2(\phi) d\phi = \frac{1}{2} A^2$$
(B.6.a.7)

$$\bar{p} = \frac{1}{2\pi} \int_0^{2\pi} m\omega A \cos(\omega t + \phi) d\phi = 0$$
(B.6.a.8)

$$\bar{p^2} = \frac{1}{2\pi} \int_0^{2\pi} m^2 \omega^2 A^2 \cos^2(\phi) d\phi = \frac{1}{2} m^2 \omega^2 A^2$$
(B.6.a.9)

(ii) We are given the expression for energy:

$$E = m\omega^2 A^2 \tag{B.6.a.10}$$

Now, we express the means in terms of energy:

$$\bar{x^2} = \frac{E}{m\omega^2} \tag{B.6.a.12}$$

$$p^2 = E \tag{B.6.a.13}$$

Next, we find the variances:

$$\Delta x^2 = \bar{x^2} - \bar{x}^2 = \frac{E}{m\omega^2}$$
 (B.6.a.14)

$$\Delta p^2 = \bar{p^2} - \bar{p}^2 = E$$
 (B.6.a.15)

B.6.b (b)

We are given the quantum operators:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}$$
(B.6.b.1)

$$\hat{a}^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}$$
(B.6.b.2)

We want to find the commutator

$$[\hat{a}, \hat{a}^{\dagger}]:$$
 (B.6.b.3)

$$[\hat{a}, \hat{a}^{\dagger}] = \hat{a}\hat{a}^{\dagger} - \hat{a}^{\dagger}\hat{a}$$
(B.6.b.4)

Using the commutation relation $[\hat{x}, \hat{p}] = i\hbar$, we find that

$$[\hat{a}, \hat{a}^{\dagger}] = 1$$
 (B.6.b.5)

Next, we rewrite the Hamiltonian in terms of \hat{a} and \hat{a}^{\dagger} :

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2$$
(B.6.b.7)

$$\hat{H} = \hbar\omega \left(\hat{a}^{\dagger} \hat{a} + \frac{1}{2} \right) \tag{B.6.b.8}$$

This is the Hamiltonian in terms of the creation and annihilation operators \hat{a}^{\dagger} and \hat{a} .

B.6.c (c)

Given the eigenvalue equation $\hat{a}^{\dagger}\hat{a}|n\rangle = n|n\rangle$, we can find $\hat{a}|n\rangle$ and $\hat{a}^{\dagger}|n\rangle$ as follows:

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$
 (B.6.c.1)

$$\hat{a}^{\dagger} \left| n \right\rangle = \sqrt{n+1} \left| n+1 \right\rangle \tag{B.6.c.2}$$

The operator \hat{a} is the annihilation (or lowering) operator, which decreases the quantum number n by 1. The operator \hat{a}^{\dagger} is the creation (or raising) operator, which increases the quantum number n by 1.

To find the ground-state wave function $\langle x|0\rangle$, we start from the eigenvalue equation for the ground state $\hat{a}|0\rangle = 0$. In the position representation, this becomes a differential equation for the wave function $\psi_0(x) = \langle x|0\rangle$:

$$\left(\sqrt{\frac{m\omega}{2\hbar}}x + \frac{i}{\sqrt{2m\hbar\omega}}\frac{d}{dx}\right)\psi_0(x) = 0$$
 (B.6.c.3)

Solving this differential equation gives the ground-state wave function up to the normalization factor N:

$$\psi_0(x) = N e^{-\frac{m\omega x^2}{2\hbar}} \tag{B.6.c.4}$$

B.6.d (d)

$$\langle x \rangle_n = \langle n | \, \hat{x} \, | n \rangle \tag{B.6.d.1}$$

$$= \langle n | \frac{1}{\sqrt{2m\hbar\omega}} (\hat{a} + \hat{a}^{\dagger}) | n \rangle$$
(B.6.d.2)

$$=\frac{1}{\sqrt{2m\hbar\omega}}(\langle n|\,\hat{a}\,|n\rangle + \langle n|\,\hat{a}^{\dagger}\,|n\rangle) \tag{B.6.d.3}$$

$$= 0 \tag{B.6.d.4}$$

To find $\left\langle x^2\right\rangle_n,$ we can use the same process as above, but with \hat{x}^2 instead of $\hat{x}:$

$$\langle x^2 \rangle_n = \langle n | \, \hat{x}^2 \, | n \rangle$$
 (B.6.d.5)

$$= \langle n | \frac{1}{2m\hbar\omega} (\hat{a} + \hat{a}^{\dagger})^2 | n \rangle$$
 (B.6.d.6)

$$=\frac{1}{2m\hbar\omega}(2n+2)\tag{B.6.d.7}$$

$$=\frac{\hbar}{m\omega}(n+\frac{1}{2}) \tag{B.6.d.8}$$

For $\langle p \rangle$, it is zero because the momentum operator does not change the state of the system, and for $\langle p^2 \rangle$, it is given by:

$$\left< p^2 \right>_n = \left< n \right| \hat{p}^2 \left| n \right> \tag{B.6.d.9}$$

$$=\hbar m\omega n \tag{B.6.d.10}$$

Using these results, we can find the variances:

$$\Delta x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{\hbar}{m\omega} (n + \frac{1}{2})$$
 (B.6.d.11)

$$\Delta p^{2} = \left\langle p^{2} \right\rangle - \left\langle p \right\rangle^{2} = \hbar m \omega n \tag{B.6.d.12}$$

Finally, we can find the product of the uncertainties:

$$\Delta x \Delta p = \sqrt{\Delta x^2 \Delta p^2} \tag{B.6.d.13}$$

$$=\sqrt{\frac{\hbar}{m\omega}(n+\frac{1}{2})}\cdot\hbar m\omega n \qquad (B.6.d.14)$$

$$=\hbar\sqrt{n(n+\frac{1}{2})}\tag{B.6.d.15}$$

$$=\hbar\sqrt{n^2 + \frac{n}{2}} \tag{B.6.d.16}$$

$$=\hbar\left(n+\frac{1}{4}\right) \tag{B.6.d.17}$$

$$=\hbar n + \frac{h}{4} \tag{B.6.d.18}$$

Finally, we can find the product of the uncertainties as applying natural units such that $c = \hbar = 1$ $1 \times n + \frac{1}{4} \ge \frac{1}{2}$. So long as *n* is positive.

B.7 7

B.7.a a

The Hamiltonian operator in cylindrical coordinates is given by:

$$\hat{H} = \frac{1}{2M} \left(\hat{p}_r^2 + \hat{p}_z^2 + \frac{\hat{L}_z^2}{r^2} \right)$$
(B.7.a.1)

where \hat{p}_z is the momentum operator in the z direction, \hat{L}_z is the angular momentum operator in the z direction, and \hat{p}_z^2 acts on a radial wavefunction as follows:

$$\langle r|\hat{p}_{z}^{2}|\psi\rangle = -\hbar\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)\langle r|\psi\rangle \tag{B.7.a.2}$$

The time-independent Schrödinger equation is given by:

$$\hat{H}|\psi\rangle = E|\psi\rangle$$
 (B.7.a.3)

Substituting the Hamiltonian operator, we get:

$$\frac{1}{2M} \left(-\hbar \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \hat{p}_z^2 + \frac{\hat{L}_z^2}{r^2} \right) |\psi\rangle = E |\psi\rangle \tag{B.7.a.4}$$

This is a partial differential equation for the wavefunction $\psi(r, \phi, z)$. The boundary conditions are that $\psi(r, \phi, z)$ must be zero at r = a and $z = \pm L/2$.

The general solution to this equation can be written as a product of functions of r, ϕ , and z:

$$\psi_{n,m}(r,\phi,z) = R_n(r)\Phi_m(\phi)Z_n(z) \tag{B.7.a.5}$$

where n and m are quantum numbers corresponding to the radial and angular momentum quantum numbers, respectively. The energy eigenvalues are given by:

$$E_{n,m} = \frac{\hbar^2}{2M} \left(\frac{n^2}{a^2} + \frac{m^2}{L^2} \right)$$
(B.7.a.6)

For L = a, the two lowest energy states correspond to (n, m) = (1, 0) and (0, 1), with energies:

$$E_{1,0} = E_{0,1} = \frac{\hbar^2}{2Ma^2} \tag{B.7.a.7}$$



Figure 5: The Four Diagrams: the real part of the wavefunction $\psi_{1,0}$ as a function of ϕ and z, and the real part of the wavefunction $\psi_{0,1}$ as a function of ϕ and z.

B.7.b b

The full wavefunction can be written as $\Psi(\vec{r}) = \psi_{n,m}(r,\phi,z)R(r)$, where $\psi_{n,m}$ are the eigenfunctions obtained in part (a) with energies $E_{n,m}$.

The time-independent Schrödinger equation becomes:

$$-\frac{\hbar^2}{2M}\nabla^2\left(\psi_{n,m}R(r)\right) = E\psi_{n,m}R(r)$$
(B.7.b.1)

Separating the variables gives us a radial equation:

$$-\frac{\hbar^2}{2M}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial R(r)}{\partial r}\right) = (E - E_{n,m})R(r)$$
(B.7.b.2)

We are told that the ground state has a form $R(r) \approx 1 - (kr)^2/4 + (kr)^4/64$ for $r \leq a$, and applying the boundary condition R(a) = 0, we get the equation:

$$1 - \frac{1}{4}(ka)^2 + \frac{1}{64}(ka)^4 = 0$$
 (B.7.b.3)

Let $x = (ka)^2$, the above equation can be rewritten as a quadratic equation:

$$64 - 16x + x^2 = 0 \tag{B.7.b.4}$$

Solving for x, we get two solutions: x = 8, 4. We discard the higher energy state x = 8, which corresponds to the first excited state, and keep the lower energy state x = 4 for the ground state. Hence, we have $k = \frac{2}{a}$.

The energy of the ground state is given by:

$$E_0 = E_{n,m} + \frac{\hbar^2 k^2}{8M}$$
(B.7.b.5)

Substituting $E_{n,m} = \frac{\hbar^2}{2Ma^2}$, the lowest energy state corresponding to (n,m) = (1,0) or (0,1), and $k = \frac{2}{a}$ into the equation, we get:

$$E_0 = \frac{\hbar^2}{2Ma^2} + \frac{\hbar^2 \left(\frac{2}{a}\right)^2}{8M} = \frac{3\hbar^2}{2Ma^2}$$
(B.7.b.6)

Thus, the ground state energy is determined in terms of a and L.

B.8 8

A particle is in a one-dimensional box with impenetrable walls at $x = \pm a$. (a) Give expressions for the normalized wavefunction and energy of the particlecin terms of the energy quantum number n and mass m.

(b) An infinitesimally thin wall at x = 0 is adiabatically introduced into the system. Taking the wall to be impenetrable once it is fully introduced, find the new normalized wavefunction and energy if the particle is initially (i) in the ground or (ii) first excited state. Infer the energy required to insert the barrier for each energy state.

(c) If the impenetrable wall is adiabatically introduced near the edge of the box, $x = a - \delta$ where $\delta < a$, sketch the resulting wavefunction for a particle initially in the ground state.

(d) Consider the case of a penetrable thin wall introduced suddenly at $\mathbf{x} = a - \delta$. If the particle is initially in the ground state, determine the probability of observing the particle in the region $a - \delta < x < a$ immediately after insertion, to lowest order in $\epsilon \equiv \frac{\delta}{2a}$ Compare the result to the classical probability. Sketch the wavefunction of the new ground state (using TikZ).

B.8.a a

For a particle in a one-dimensional box with impenetrable walls at $x = \pm a$, we can use the solutions to the time-independent Schrödinger equation. The wavefunction is given by:

$$\psi_n(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi(x+a)}{2a}\right)$$
(B.8.a.1)

This is a sinusoidal wavefunction that is normalized, i.e., its integral over the entire box is equal to 1. The energy of the particle is given by:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{8ma^2}$$
(B.8.a.2)

Where n is a positive integer and represents the energy quantum number, m is the mass of the particle, and \hbar is the reduced Planck constant.

B.8.b b

When an infinitesimally thin wall is adiabatically introduced at x = 0, the particle is effectively confined to two separate boxes of length a. For each box, the wavefunction is now given by:

$$\psi_n^+(x) = \begin{cases} \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{2a}\right), & \text{for } x \in [-a, 0] \\ \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi (x-a)}{2a}\right), & \text{for } x \in [0, a] \end{cases}$$
(B.8.b.1)

The energy levels for the new system are given by:

$$E_n^+ = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$
(B.8.b.2)

The energy difference for the ground state (n = 1) and the first excited state (n = 2) can be calculated:

$$\Delta E_1 = E_1^+ - E_1 = \frac{3\hbar^2 \pi^2}{8ma^2}$$
(B.8.b.3)

$$\Delta E_2 = E_2^+ - E_2 = 0 \tag{B.8.b.4}$$





Figure 6: Impenetrable Barrier

When an impenetrable wall is adiabatically introduced near the edge of the box at $x = a - \delta$, where $\delta < a$, the particle is effectively confined to a smaller box of length $a - \delta$. The wavefunction of the particle, initially in the ground state, is given by $\sqrt{\frac{2}{a}} \sin\left(\frac{\pi(x+a)}{2a}\right)$ for $x \in [-a, a-\delta]$ and is zero for $x \in [a-\delta, a]$. This is a sine function that satisfies the boundary conditions at x = -a, $x = a - \delta$, and x = a. The plot shows the wavefunction of the particle as a function of position, with the position of the wall indicated by a red dashed line. The wavefunction is zero at the location of the wall and beyond, indicating that the particle cannot exist there due to the impenetrable barrier.

B.8.d d

For a penetrable thin wall introduced suddenly at $x = a - \delta$, we can use perturbation theory to find the probability of observing the particle in the region $a - \delta < x < a$ immediately after insertion. To lowest order in $\epsilon \equiv \frac{\delta}{2a}$, we can find the first-order correction to the ground state energy:

$$\Delta E_1^{(1)} = \langle \psi_1 | V | \psi_1 \rangle = V_0 \int_{a-\delta}^a \psi_1^2(x) dx$$
 (B.8.d.1)

Where V_0 is the potential of the wall and $\psi_1(x)$ is the wavefunction of the ground state. We can approximate this integral by noting that $\psi_1(x)$ is nearly constant over the small region $a - \delta < x < a$. Thus, the probability of finding the particle in the region $a - \delta < x < a$ is:

$$P = \int_{a-\delta}^{a} \psi_1^2(x) dx \approx \psi_1^2(a-\delta)\delta$$
(B.8.d.2)

$$= \left[\sqrt{\frac{1}{a}}\sin\left(\frac{\pi(a-\delta+a)}{2a}\right)\right]^2\delta \tag{B.8.d.3}$$

$$=\sin^2\left(\frac{\pi}{2} - \frac{\pi\delta}{2a}\right)\delta\tag{B.8.d.4}$$

$$\approx \sin^2(\pi\epsilon)\delta$$
 (B.8.d.5)

$$\approx \pi^2 \epsilon^2 \delta$$
 (B.8.d.6)

Comparing this to the classical probability, which would be $\frac{\delta}{2a} = \epsilon$, we see that the quantum probability is larger by a factor of $\pi^2 \epsilon$. To sketch the wavefunction of the new ground state, we can observe that the wavefunction will be nearly unchanged except near the wall, where it will be slightly perturbed.



Figure 7: Penetrable Barrier