

UNIVERSITY OF ALABAMA
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PH 253 / LeClair

Spring 2010

Exam 2 Sample Problems

1. The wavefunction of a particle in a double slit experiment with slit spacing d and slit width $w < d$ (w, d both positive quantities) in the plane of the slits is described by

$$\psi(x) = \begin{cases} C & -\frac{d}{2} - \frac{w}{2} \leq x \leq -\frac{d}{2} + \frac{w}{2} & \text{(slit a)} \\ C & \frac{d}{2} - \frac{w}{2} \leq x \leq \frac{d}{2} + \frac{w}{2} & \text{(slit b)} \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

(a) Determine the normalization constant C .

(b) Determine $\langle x \rangle$ and $\langle x^2 \rangle$ in the limit $w \ll d$, i.e., ignore any terms of order w/d and higher in the end result.

(c) Again for $w \ll d$, find the uncertainty in position $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$.

Solution: We can normalize the wavefunction by integrating its square over all space and setting the result equal to 1. This enforces that the particle has unit probability of being *somewhere*.

$$\int |\psi(x)|^2 dx = \int_{-\frac{d}{2}-\frac{w}{2}}^{-\frac{d}{2}+\frac{w}{2}} C^2 dx + \int_{\frac{d}{2}-\frac{w}{2}}^{\frac{d}{2}+\frac{w}{2}} C^2 dx = C^2 w + C^2 w = 2wC^2 = 1 \quad (2)$$

$$\implies C = \frac{1}{\sqrt{2w}} \quad (3)$$

Finding $\langle x \rangle$ is not much harder, in principle.

$$\begin{aligned} \langle x \rangle &= \int x |\psi(x)|^2 dx = \int_{-\frac{d}{2}-\frac{w}{2}}^{-\frac{d}{2}+\frac{w}{2}} x C^2 dx + \int_{\frac{d}{2}-\frac{w}{2}}^{\frac{d}{2}+\frac{w}{2}} x C^2 dx = \frac{1}{2} C^2 x^2 \Big|_{-\frac{d}{2}-\frac{w}{2}}^{-\frac{d}{2}+\frac{w}{2}} + \frac{1}{2} C^2 x^2 \Big|_{\frac{d}{2}-\frac{w}{2}}^{\frac{d}{2}+\frac{w}{2}} \\ &= \frac{1}{2} C^2 \left[\left(-\frac{d}{2} + \frac{w}{2} \right)^2 - \left(-\frac{d}{2} - \frac{w}{2} \right)^2 \right] + \frac{1}{2} C^2 \left[\left(\frac{d}{2} + \frac{w}{2} \right)^2 - \left(\frac{d}{2} - \frac{w}{2} \right)^2 \right] \\ &= \frac{1}{2} C^2 \left[\frac{d^2}{4} - \frac{dw}{2} + \frac{w^2}{4} - \frac{d^2}{4} - \frac{dw}{2} - \frac{w^2}{4} \right] + \frac{1}{2} C^2 \left[\frac{d^2}{4} + \frac{dw}{2} + \frac{w^2}{4} - \frac{d^2}{4} + \frac{dw}{2} - \frac{w^2}{4} \right] \\ &= \frac{1}{2} C^2 [-dw] + \frac{1}{2} C^2 [dw] = 0 \end{aligned} \quad (4)$$

Of course, since the integrand is an odd function of x and the integration limits are symmetric, we could have seen that $\langle x \rangle$ must be zero just based on symmetry. Finding $\langle x^2 \rangle$ we have no such trick to make use of ...

$$\begin{aligned} \langle x^2 \rangle &= \int x^2 |\psi(x)|^2 dx = \int_{-d/2-w/2}^{-d/2+w/2} x^2 C^2 dx + \int_{d/2-w/2}^{d/2+w/2} x^2 C^2 dx = \frac{1}{3} C^2 x^3 \Big|_{-d/2-w/2}^{-d/2+w/2} + \frac{1}{3} C^2 x^3 \Big|_{d/2-w/2}^{d/2+w/2} \\ &= \frac{1}{3} C^2 \left[\left(-\frac{d}{2} + \frac{w}{2} \right)^3 - \left(-\frac{d}{2} - \frac{w}{2} \right)^3 \right] + \frac{1}{3} C^2 \left[\left(\frac{d}{2} + \frac{w}{2} \right)^3 - \left(\frac{d}{2} - \frac{w}{2} \right)^3 \right] \end{aligned} \quad (5)$$

At this point, we have a great many terms to evaluate. However, since we need only terms of first order in w/d , we can divide out a factor $d^3/2^3$ and simplify by taking only the first terms in the expansion:

$$\begin{aligned} \langle x^2 \rangle &= \frac{1}{24} C^2 d^3 \left[\left(-1 + \frac{w}{d} \right)^3 + \left(1 + \frac{w}{d} \right)^3 + \left(1 + \frac{w}{d} \right)^3 - \left(1 - \frac{w}{d} \right)^3 \right] \\ &= \frac{1}{12} C^2 d^3 \left[\left(1 + \frac{w}{d} \right)^3 - \left(1 - \frac{w}{d} \right)^3 \right] \approx \frac{1}{12} C^2 d^3 \left[1 + 3\frac{w}{d} - 1 + 3\frac{w}{d} \right] \\ &= \frac{1}{2} C^2 d^2 w = \frac{1}{2} \left(\frac{1}{2w} \right) d^2 w = \frac{1}{4} d^2 \end{aligned} \quad (6)$$

Finally,

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{1}{4} d^2 - 0} = \pm \frac{1}{2} d \quad (7)$$

2. The state of a free particle is described by the following wave function

$$\psi(x) = \begin{cases} 0 & x < -b \\ A & -b \leq x \leq 3b \\ 0 & x > 3b \end{cases} \quad (8)$$

- (a) Determine the normalization constant A .
- (b) What is the probability of finding the particle in the interval $[0, b]$?
- (c) Determine $\langle x \rangle$ and $\langle x^2 \rangle$ for this state.
- (d) Find the uncertainty in position $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$.

Solution: As above, we can normalize the wavefunction by integrating its square over all space.

Conveniently, the wavefunction is zero except over the interval $[-b, 3b]$

$$\int |\psi(x)|^2 dx = \int_{-b}^{3b} A^2 dx = 4bA^2 = 1 \quad \implies \quad A = \frac{1}{2\sqrt{b}} \quad (9)$$

The probability of finding the particle in $[0, b]$ means integrating the probability density, $|\psi|^2$ over that interval:

$$P(x \in [0, b]) = \int_0^b A^2 dx = \int_0^b \frac{1}{4b} dx = \frac{1}{4} \quad (10)$$

Finding $\langle x \rangle$ proceeds as above, though now the integration interval is asymmetric, and we expect a nonzero value:

$$\langle x \rangle = \int_{-b}^{3b} \frac{x}{4b} dx = \frac{1}{4b} \left[\frac{1}{2} x^2 \right]_{-b}^{3b} = \frac{1}{8b} (9b^2 - b^2) = b \quad (11)$$

Similarly,

$$\langle x^2 \rangle = \int_{-b}^{3b} \frac{x^2}{4b} dx = \frac{1}{12b} [x^3]_{-b}^{3b} = \frac{1}{12b} [27b^3 + b^3] = \frac{7}{3} b^2 \quad (12)$$

Thus,

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{7}{3} b^2 - b^2} = \pm \frac{2b}{\sqrt{3}} \quad (13)$$

3. The hydrogen 1s wavefunction is

$$\psi_{1s} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \quad (14)$$

(a) Find the most probable distance from the origin to find an electron. (a_0)

(Hint: maximize $P(r) = 4\pi r^2 |\psi|^2$.)

(b) Find the expected distance from the origin, $\langle r \rangle$. ($\frac{3}{2} a_0$) Note

$$\int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$$

Solution: The probability of finding an electron at radius r in the interval $[r, r + dr]$ is

$$P(r) = 4\pi r^2 |\psi|^2 = \frac{4r^2}{a_0^3} e^{-2r/a_0} \quad (15)$$

Thus, the maximum probability occurs when

$$\frac{dP}{dr} = 0 = \frac{8r}{a_0^3} e^{-2r/a_0} - \frac{8r^2}{a_0^4} e^{-2r/a_0} \quad (16)$$

$$0 = \frac{8r^2}{a_0^3} - \frac{8r^2}{a_0^4} \quad (17)$$

$$0 = 1 - \frac{r}{a_0} \quad (18)$$

$$r = a_0 \quad (19)$$

The expected value of r is found via

$$\langle r \rangle = \int_0^{\infty} rP(r) dr = \int_0^{\infty} \frac{4r^3}{a_0^3} e^{-2r/a_0} dr = \frac{4}{a_0^3} \frac{3!}{(2/a_0)^4} = \frac{24}{a_0^3} \frac{a_0^4}{16} = \frac{3}{2} a_0 \quad (20)$$

Here we used the given integral for $n=3$.

4. How many different photons can be emitted by hydrogen atoms that undergo transitions to the ground state from the $n=5$ state? Enumerate their energies. (Hint: draw an energy level diagram, and remember that the level spacing is *not* equal. Answer: 10.)

Solution: All states from $n=5$ to $n=1$ have different energies, and their spacing is not equal. Thus, we have the following possible transitions to the ground state:

$5 \rightarrow 1$
 $5 \rightarrow 4, 4 \rightarrow 1$
 $5 \rightarrow 4, 4 \rightarrow 3, 3 \rightarrow 1$
 $5 \rightarrow 4, 4 \rightarrow 3, 3 \rightarrow 2, 2 \rightarrow 1$
 $5 \rightarrow 4, 4 \rightarrow 2, 2 \rightarrow 1$
 $5 \rightarrow 3, 3 \rightarrow 1$
 $5 \rightarrow 3, 3 \rightarrow 2, 2 \rightarrow 1$
 $5 \rightarrow 2, 2 \rightarrow 1$

The different photons that can be emitted correspond to the unique level transitions above:

$5 \rightarrow 4, 5 \rightarrow 3, 5 \rightarrow 2, 5 \rightarrow 1$
 $4 \rightarrow 3, 4 \rightarrow 2, 4 \rightarrow 1$
 $3 \rightarrow 2, 3 \rightarrow 1$
 $2 \rightarrow 1$

Thus, there are 10 possible transitions, and the energy differences are calculated according to the Bohr model

$$\Delta E_{nn'} = -13.6 \text{ eV} \left(\frac{1}{n^2} - \frac{1}{n'^2} \right) \quad (21)$$

where n and n' are the numbers of the initial and final states, respectively.

5. Electrons of energy 12.2 eV are fired at hydrogen atoms in a gas discharge tube. Determine the wavelengths of the lines that can be emitted by the hydrogen. *Hint: to what state can the hydrogen atom be excited, given an excess energy of 12.2 eV above its ground state?* (Answer: 656.3, 121.5, 102.6 nm)

Solution: If the hydrogen atom is in its ground state, it has an energy of -13.6 eV . Giving it another 12.2 eV means it has an energy of -1.4 eV , and the maximum state it can be excited to is thus

$$-1.4 \text{ eV} = \frac{-13.6 \text{ eV}}{n^2} \quad (22)$$

This gives $n=3.1$, so the atom may be excited to the $n=3$ state (the $n=4$ state has an energy of

−0.85 eV, and cannot be reached). The hydrogen atom may then relax to the ground state from the third state by the following paths:

$$3 \rightarrow 1$$

$$3 \rightarrow 2, 2 \rightarrow 1$$

This gives us three possible photon energies:

$$E_3 - E_1 = -13.6 \text{ eV} \left(\frac{1}{3^2} - \frac{1}{1^2} \right) = 12.09 \text{ eV}$$

$$E_3 - E_2 = -13.6 \text{ eV} \left(\frac{1}{3^2} - \frac{1}{2^2} \right) = 1.88 \text{ eV}$$

$$E_2 - E_1 = -13.6 \text{ eV} \left(\frac{1}{2^2} - \frac{1}{1^2} \right) = 10.2 \text{ eV}$$

The photon wavelengths are then given by $\lambda = hc/\Delta E \approx 1240 \text{ eV} \cdot \text{nm}/\Delta E$ for

$$\lambda = \{659.6, 121.5, 102.6\} \text{ nm} \tag{23}$$

6. Determine the correction to the wavelength of an emitted photon when the recoil kinetic energy of the hydrogen nucleus is taken into account. (Hint: use conservation of energy and momentum. Fractional change $\sim 10^{-9}$)

Solution: Assuming that the atom is initially at rest, conservation of energy gives

$$E_i = E_f + E_\gamma + K \tag{24}$$

Here E_i is the initial and E_f the final energy of the atom, E_γ is the photon energy, and K the recoil kinetic energy of the nucleus. Neglecting the nuclear recoil correction, this would simply give $E_f - E_i = E_\gamma = \frac{hc}{\lambda_0}$ as we are used to, giving a photon wavelength λ_0 . Rearranging,

$$\frac{E_i - E_f}{hc} - \frac{E_\gamma}{hc} = \frac{K}{hc} \tag{25}$$

The first term on the left would be the wavelength neglecting the nuclear recoil correction, $1/\lambda_0$, while the second gives the actual corrected wavelength $1/\lambda$:

$$\frac{1}{\lambda_0} - \frac{1}{\lambda} = \frac{K}{hc} \tag{26}$$

In terms of a fractional correction,

$$\frac{\lambda - \lambda_0}{\lambda_0} = \frac{\lambda K}{hc} \quad (27)$$

The recoil momentum of the nucleus will be $p = \sqrt{2MK}$, where M is the nuclear mass.ⁱ Conservation of momentum between the recoiling nucleus and the exiting photon gives

$$0 = \sqrt{2MK} - \frac{h}{\lambda} \quad \implies \quad K = \frac{h^2}{2M\lambda^2} \quad (28)$$

Thus,

$$\frac{\lambda - \lambda_0}{\lambda_0} = \frac{\lambda (h^2/2M\lambda^2)}{hc} = \frac{hc}{2(Mc^2)\lambda} \approx \frac{6.6 \times 10^{-7} \text{ nm}}{\lambda} \quad (29)$$

For hydrogen, the wavelengths of the lowest transitions are on the order of 10^2 nm, so the fractional change is on the order of 10^{-9} , and thus utterly negligible.

7. Show that whenever a solution $\Psi(x, t)$ of the time-dependent Schrödinger equation separates into a product $\Psi(x, t) = F(x) \cdot G(t)$ then $F(x)$ *must* satisfy the corresponding time-independent Schrödinger equation and $G(t)$ *must* be proportional to $e^{-iEt/\hbar}$.

Solution: The time-dependent Schrödinger equation reads

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi \quad (30)$$

Where \hat{H} represents the kinetic plus potential energy,

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \quad (31)$$

Substituting our separated solution, and noting that any spatial derivative of $G(t)$ is zero,

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2 F(x)}{\partial x^2} + V(x)F(x) \right) G(t) = i\hbar F(x) \frac{\partial G(t)}{\partial t} \quad (32)$$

Separate everything that depends on x to the left, and everything that depends on t to the right:

$$\frac{-\frac{\hbar^2}{2m} \frac{\partial^2 F(x)}{\partial x^2} + V(x)F(x)}{F(x)} = \frac{i\hbar \frac{\partial G(t)}{\partial t}}{G(t)} \quad (33)$$

ⁱSince $K = p^2/2m$.

If both sides are equal, then they must both be equal to the same constant value, which we will denote as E . Thus,

$$\frac{-\hbar^2}{2m} \frac{\partial^2 F(x)}{\partial x^2} + V(x)F(x) = EF(x) \quad (34)$$

Thus, $F(x)$ obeys the time-independent Schrödinger equation. Further,

$$i\hbar \frac{\partial G(t)}{\partial t} = EG(t) \quad (35)$$

The latter equation can be re-written

$$\frac{\partial G(t)}{\partial t} = \frac{E}{i\hbar} G(t) = -\frac{iE}{\hbar} G(t) \quad (36)$$

which has the general solutionⁱⁱ

$$G(t) = Ce^{-iEt/\hbar} \quad (37)$$

NB: this is probably not something I would ask on the exam, as it is more math than physics.

8. A particle is in a stationary state in the potential $V(x)$. The potential function is now increased over all x by a constant value V_o . What is the effect on the quantized energy? Show that the spatial wave function of the particle remains unchanged. (Answer: all energies raised by V_o .)

Solution: Changing the overall value of the potential by V_o is equivalent to changing the zero of potential energy by V_o . Since we can only measure differences in potential energy, all this does is globally shift our energy readings by V_o , and the measured energies must also then increase by V_o . The time-independent Schrödinger equation in 1D reads

$$E\psi = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \quad (38)$$

Adding V_o to the potential energy gives

$$E\psi = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + (V(x) + V_o)\psi \quad (39)$$

$$(E - V_o)\psi = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \quad (40)$$

$$(41)$$

ⁱⁱRecall that if $-a \frac{dy}{dx} = y$, the general solution is $y = Ce^{-t/a}$, where C is a constant.

Thus, the same time-independent Schrödinger equation is obeyed, with the energies are shifted upward by V_0 . The spatial part of the wave function remains unchanged, since $\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi$ is still just equal to a constant times ψ .

9. An experimenter asks for funds from a foundation to observe visually through a microscope the quantum behavior of a small harmonic oscillator. According to his proposal, the oscillator consists of an object 10^{-6} m in diameter and estimated mass of 10^{-15} kg. It vibrates on the end of a thin fiber with a maximum amplitude of 10^{-5} m and frequency 1000 Hz. You are the referee for the proposal.

(a) What is the approximate quantum number for the system in the state described? (About 3×10^{12} .)

(b) What would its energy be in electron volts if it were in its lowest energy state? Compare with the average thermal energy at room temperature, $\sim 1/40$ eV. (About 2×10^{-12} eV.)

(c) What would its classical amplitude of vibration be if it were in its lowest energy state? Compare with the wavelength of visible light, about 500 nm, with which it is presumably observed. (About 4×10^{-12} m.)

(d) Would you, as a referee of this proposal, recommend award of a grant to carry out this research? (No!)

Solution: The energy of a quantum simple harmonic oscillator can be written in terms of its frequency f , its principle quantum number n , and Planck's constant h :

$$E = \left(n + \frac{1}{2} \right) hf \quad (42)$$

If the object is a mechanical oscillator, then its vibrational energy must also be related to its amplitude of vibration A :

$$E = \frac{1}{2}kA^2 \quad \text{with} \quad 2\pi f = \sqrt{\frac{k}{m}} \quad (43)$$

here k is the effective spring constant and m the mass of the oscillator. Combining the last two expressions, and using the quantities given, we have

$$\left(n + \frac{1}{2} \right) hf = 2\pi^2 m f^2 A^2 \quad (44)$$

$$n = \frac{2\pi^2 m}{h} f A^2 - \frac{1}{2} \approx \frac{2\pi^2 m}{h} f A^2 \approx 3 \times 10^{12} \quad (45)$$

The system is in a *very* high quantum state, far too high to expect to observe any discretization of vibrational modes – this would require a precision of ~ 1 part in 10^{12} in frequency measurement. Its

energy in electron volts for the lowest state, $n=0$, may then be calculated from either expression:

$$E_0 = \left(0 + \frac{1}{2}\right) hf \approx 3 \times 10^{-31} \text{ J} \approx 2 \times 10^{-12} \text{ eV} \quad (46)$$

Clearly, the thermal energy at room temperature will induce an overwhelming random vibration. The amplitude of vibration can be determined by inverting the expression for energy above:

$$A = \frac{1}{\pi f} \sqrt{\frac{E}{2m}} \approx 4 \times 10^{-12} \text{ m} = 4 \times 10^{-3} \text{ nm} \quad (47)$$

This is roughly five orders of magnitude smaller than the wavelength of light, definitively precluding any optical observation. Very hard X-rays would be required, and at a wavelength of 10^{-12} m , the photon energy would be about 1 MeV, more than sufficient to disturb the oscillator. We cannot recommend funding of this project!

10. The molecular bonding in the compound NaCl is predominantly ionic, and to a good approximation we can consider a sodium chloride molecule as consisting of two units – an Na^+ ion and a Cl^- ion – bound together. Assuming an electrostatic attraction and a power-law repulsion between the ions, their potential energy as a function of ion spacing has the form

$$V(r) = -\frac{ke^2}{r} + \frac{A}{r^n} \quad (48)$$

- (a) Find the equilibrium spacing r_o .
- (b) Find the potential energy at this separation, V_{\min} .
- (c) Find the effective “spring constant” for the molecule, assuming small deviations from r_o . One way to do this is to find the second derivative of $V(r)$ at $r=r_o$. $[(n-1)ke^2/r_o^3]$

Solution: Equilibrium spacing occurs when $dV/dr=0$:

$$\left. \frac{dV}{dr} \right|_{r_o} = \frac{ke^2}{r_o^2} - \frac{nA}{r_o^{n+1}} = 0 \quad (49)$$

$$ke^2 = \frac{nA}{r_o^{n-1}} \quad (50)$$

$$r_o = \left(\frac{nA}{ke^2} \right)^{1/(n-1)} \quad (51)$$

At this separation, we have

$$V(r_o) = -\frac{ke^2 (ke^2)^{1/(n-1)}}{(nA)^{1/(n-1)}} + \frac{A (ke^2)^{n/(n-1)}}{(nA)^{n/(n-1)}} = -\frac{(ke^2)^{n/(n-1)}}{(nA)^{1/(n-1)}} + A \left(\frac{ke^2}{nA}\right)^{n/(n-1)} \quad (52)$$

$$= (ke^2)^{n/(n-1)} \left(\frac{1}{(nA)^{1/(n-1)}} + \frac{A}{(nA)^{n/(n-1)}} \right) \quad (53)$$

$$= (ke^2)^{n/(n-1)} \left(\frac{1}{(nA)^{1/(n-1)}} + \frac{1}{n(nA)^{1/(n-1)}} \right) = \left(\frac{k^n e^{2n}}{nA} \right)^{1/(n-1)} \left(1 + \frac{1}{n} \right) \quad (54)$$

The spring constant can be found by approximating d^2V/dr^2 as constant near r_o :

$$\left. \frac{d^2V}{dr^2} \right|_{r_o} = -\frac{2ke^2}{r_o^3} + \frac{n(n+1)A}{r_o^{n+2}} = -2ke^2 \left(\frac{ke^2}{nA} \right)^{3/(n-1)} + n(n+1)A \left(\frac{ke^2}{nA} \right)^{(n+2)/(n-1)} \quad (55)$$