Physics 215B- Quantum Mechanics, Winter 2014

Problem Set 3, due Tuesday February 4

[**1.**] A free particle of mass m is "prepared" so that it is in the plane wave state $e^{i\vec{k}\cdot\vec{r}}$ with $\vec{k} = k\hat{z}$. What will a measurement of $\hat{H} = \hat{p}^2/2m$ find? What will a measurement of $\hat{L}^2$ or $\hat{L}_z$ find? (Give the possible answers and their probabilities.) In what states will these measurements leave the system?

[**2.**] A "quantum dot," relevant to semiconductor devices, may be modeled as an electron in an infinite spherical well. Design a quantum dot whose characteristic frequency of emission is 10 GHz, where "characteristic frequency" corresponds to decay from the first excited to the ground state. That is, obtain the radius a of the well which has this property. Repeat the problem for a quantum dot which has the shape of a cube. In either case, assume the mass of the "effective mass" of the electron is $m = 0.067m_e$. (All this means is that electrons in semiconductors behave as if their mass is different from the mass of an electron in vacuum.)

[**3.**] Solve the equation $df/dx + f = 0$ by the series expansion technique.

[**4.**] In classical physics two particles interacting with a central force can be recast as a single particle particle problem by introducing relative and center of mass variables. Discuss whether this can be done, and provide details if it can be accomplished, in quantum mechanics. (This exercise is asking whether it made sense for us to do the hydrogen atom ignoring the fact that the proton can move.)

Physics 215B Winter 2014

Problem Set # 3.

$\boxed{1}$ As discussed in class, this problem is ill-posed because the given wave function is not normalizable.

Let's do as much as we can and discuss what makes sense qualitatively about things we find.

First, $e^{i\vec{k}\cdot\vec{r}} = e^{ikz}$ is an eigenstate of $\hat{p}$ and hence of $\hat{H} = \hat{p}^2/2m$. We get a definite value for measuring $\hat{H}$ (E) of $\hbar^2 k^2/2m$.

Next we recall

$$e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, P_l(\cos\theta)$$

$$Y_{l0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta)$$

where $z = r\cos\theta$.

1 (cont'd)

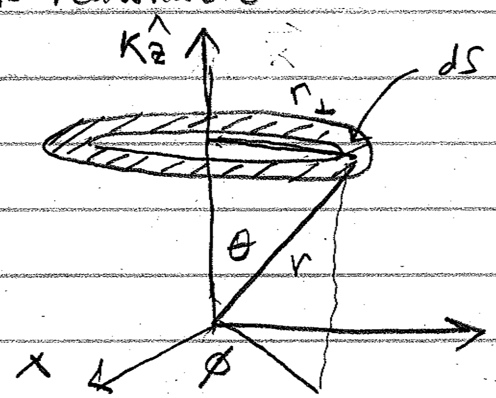
Since only $Y_{\ell m}$ with $m=0$ appear in the expansion of e^{ikz} we are <u>guaranteed</u> to measure $\emptyset$ for $\hat{L}_z$

This is physically reasonable since the plane wave moving in the $\hat{z}$ direction has no sense of rotation about the $\hat{z}$ axis.

The probability of measuring $\ell(\ell+1)\hbar^2$ for $\hat{L}^2$ is given by the square of the coefficient of $P_\ell(\cos\theta)$ from the usual rules of measurement. In particular it will grow as $(2\ell+1)^2$. Here we have trouble because we cannot do the sum $\sum_{\ell=0}^{\infty}(2\ell+1)^2$ to normalize.

Nevertheless we can argue physically why the result is reasonable?

with $\psi \sim e^{ikz}$ $|\psi|^2 \sim 1$ particle equally likely to be <u>anywhere</u>



$dS = 2\pi\, r_\perp\, dr_\perp = \pi\, d(r_\perp^2)$

particles in this region of space have the same $\ell = r_\perp \hbar k$

1 (cont'd) Since prob of having $r_\perp$ grows as $d(r_\perp)^2$ and since $\ell \sim r_\perp$ we see prob of having $\ell \sim d(\ell^2)$ which is in agreement with our $(2\ell+1)^2 \sim \ell^2$ result.

To make this problem really work, one might try

$$\psi(r,\theta,\phi) = N e^{-r^2/a^2} e^{ikz}$$

which would be normalizable. The question is whether it is simple to expand such a function in terms of $j_\ell(kr)$ and $Y_{\ell m}(\theta,\phi)$. I guess it's obvious that only $Y_{\ell 0}(\theta,\phi)$ will enter, since e^{-r^2/a^2} has no ϕ dependence.

One can probably use properties of j_ℓ to make some rough predictions for the probability of getting $\ell(\ell+1)\hbar^2$ for $\hat{L}^2$. Thinking physically e^{-r^2/a^2} kills off r values greater than a, so it would be pretty unlikely to get $\ell \gtrsim a\hbar k$

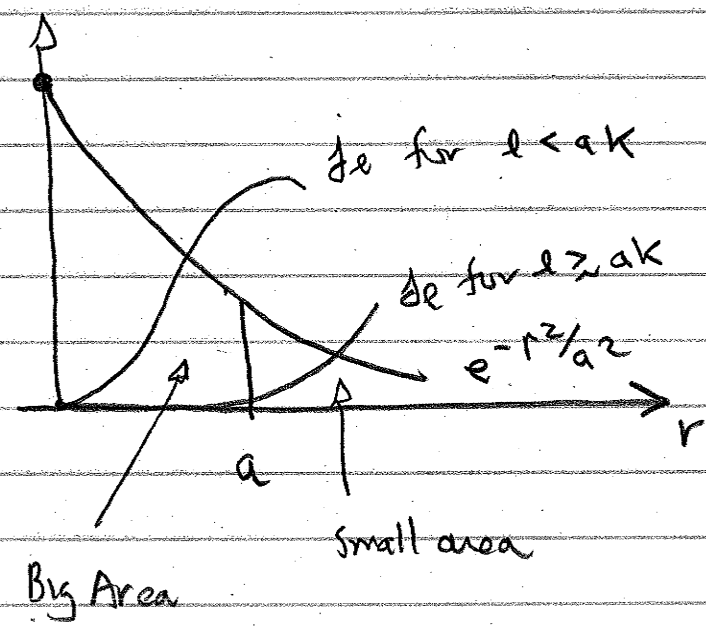
Thus I am pretty sure one will find

$$\text{prob}(\ell) \sim 0 \quad \text{for} \quad \ell \gtrsim ak$$

This will make $\sum_\ell p(\ell)$ converge and normalizable.

Can one see from plotting $j_\ell(r)$ that the area under $j_\ell(r)\, e^{-r^2/a^2}$ gets tiny when $\ell \gtrsim ak$?

eg



$\boxed{2}$ Let's do the easier case of a cubic dot first.

Actually, that already makes the main point of the problem, which is to get a rough idea of how big a quantum dot needs to be to radiate at 10 GHz.

$$E(n_x n_y n_z) = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2\left[n_x^2 + n_y^2 + n_z^2\right]$$

Ground state $n_x = n_y = n_z = 1$

First excited state $n_x = 2 \quad n_y = 1 \quad n_z = 1$

$$\therefore \Delta E = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2\left\{(2^2+1^2+1^2) - (1^2+1^2+1^2)\right\}$$

$$= 3\hbar^2/2m \left(\pi/a\right)^2$$

We want this to equal $\hbar\, 10^{10}$ ← 10 GHz at $m_e = 0.067\, m_e$

$$3\hbar^2/2m \left(\pi/a\right)^2 = \hbar\, 10^{10}$$

$$\text{whence} \quad a = \left(\frac{3\hbar\ \pi^2}{2(.067 m_e)}\frac{1}{10^{10}}\right)^{1/2} = 1.6 \cdot 10^{-6}\ m$$

$\hbar = 1.06 \cdot 10^{-34}$

$m_e = 9.11 \cdot 10^{-31}$

We can check this number as follows: we know the Hydrogen atom size is roughly a Bohr radius $a_0 \sim .5 \cdot 10^{-10}$ m and that its transitions are in the range of visible light $f \sim 10^{15}$ $\omega \sim 10^{16}$

since the energy levels $\sim 1/\ell^2$ where ℓ is size of system, we can estimate

$$a \sim \underbrace{.5 \cdot 10^{-8}}_{a_0} \sqrt{10^{16}/10^{10}} \sim .5 \cdot 10^{-5} = 5 \cdot 10^{-6} m$$

This estimate is within a factor of 3 of the value on page 2-1. Actually we have been a bit sloppy here. The Bohr radius is computed using $m = m_e$ not $m = .067\, m_e$. Since $a \sim m^{-1/2}$ we really should reduce this value by $(.067)^{-1/2} = 3.9$ which brings us into even better agreement with 2-1.

12/cont'd Finally let's tackle the ∞ spherical well problem. The energy levels are

$$E_{n\ell} = \frac{\hbar^2}{2ma^2}\beta_{n\ell}^2$$

where $\beta_{n\ell}$ is the nth root of the spherical Bessel function j_ℓ

Some of these are:

(n,ℓ)	1,0	1,1	1,2	2,0	1,3	2,1
$\beta_{n\ell}$	π	4.49	5.76	2π	6.99	7.73

The first excited state to ground state transition is at

$$\frac{\hbar^2}{2ma^2}\left\{4.49^2 - \pi^2\right\} = \hbar\, 10^{10}$$

which gives $a = \left[\dfrac{\hbar\,(4.49^2 - \pi^2)}{2(.067\, m_e)\, 10^{10}}\right]^{1/2}$

$$= 0.9 \cdot 10^{-6}\ m$$

So this is in the same ball park as 2-2 and 2-1

A good "rule of thumb" is that a QM particle confined in a region of size ℓ has energy $\dfrac{\hbar^2}{2m}\dfrac{1}{\ell^2}$

3-1

In solving H atom radial eqn to get Laguerre polynomials we try a series sol'n guess. The purpose of this problem is to illustrate the technique in a more simple setting

$$df/dx + f = 0$$

guess $\quad f = \sum_{q=0}^{\infty} c_q x^q$

$$\rightarrow \quad \sum_{0}^{\infty} q c_q x^{q-1} + \sum_{0}^{\infty} c_q x^q = 0$$

$$\hookrightarrow \sum_{-1}^{\infty} (q+1) c_{q+1} x^q$$

NB first term is zero.

Insisting sum varies term by term

$$(q+1) c_{q+1} + c_q = 0$$

recursion rel'n similar to what we found for H-atom

$$c_{q+1} = -c_q/_{q+1}$$

$$\rightarrow \quad c_1 = -c_0/_1 \qquad c_2 = -c_1/_2 = +c_0/_2 \qquad c_3 = -c_2/_3 = -c_0/_6$$

$$\rightarrow \quad c_q = c_0/_{q!} (-1)^q \qquad f = c_0 \sum x^q/_{q!} (-1)^q = c_0 e^{-x}$$

So we get expected result

10.35

Let's review how a classical 2 body central force problem reduces to 1 body.

$$E = p_1^2/2m_1 + p_2^2/2m_2 + V(r_1 - r_2)$$

We introduce center of mass and relative coordinates

$$\left.\begin{array}{l} R = (m_1 r_1 + m_2 r_2)/m_1+m_2 \\ \underline{P} = p_1 + p_2 \end{array}\right\} \quad M = m_1 + m_2$$

$$\left.\begin{array}{l} r = r_1 - r_2 \\ p = m_2 p_1 - m_1 p_2 / m_1 + m_2 \end{array}\right\} \quad \mu = m_1 m_2 / m_1 + m_2$$

The latter eqn is less familiar but it is what is needed for

$$p_1^2/2m_1 + p_2^2/2m_2 = p^2/2\mu + \underline{P}^2/2M$$

Let's check (forget common factor of 2!)

$$p^2/\mu + \underline{P}^2/M = \frac{(m_2 p_1 - m_1 p_2)^2}{(m_1+m_2)^2} \frac{(m_1+m_2)}{m_1 m_2} + \frac{(p_1+p_2)^2}{m_1+m_2}$$

Cross terms $(p_1 p_2)$: $\quad -2/(m_1+m_2) \quad + 2/(m_1+m_2)$ ✓✓

p_1^2 term $\quad m_2/m_1(m_1+m_2) + 1/m_1+m_2 = 1/m_1$ ✓✓

(~~p_2^2 term is same by~~ symmetry)

It is also true that $l_1 + l_2 = l + L$

where $l_1 = r_1 \times p_1$ $\qquad l = r \times p$

$l_2 = r_2 \times p_2$ $\qquad L = R \times P$

Since $E = \dfrac{P^2}{2M} + p^2/2\mu + V(r)$

has no R dependence $\quad \dot{P} = 0$ (cm momentum conserved)

$\dot{p} = -\nabla V(r)$ ← a 1 body problem

* Now turn to QM. The change of variables is identical

The most impt thing to verify, as you might expect

are the commutation relations. For example,

$$[r_j, P_k] = [r_{1j} - r_{2j}, (m_2 P_{1k} - m_1 P_{2k})/m_1 + m_2]$$

Note operators associated with particles 1+2 commute. →

$$= \frac{1}{m_1+m_2}\Big(m_2 \underbrace{[r_{1j}, p_{1k}]}_{i\hbar\delta_{jk}} + m_1 \underbrace{[r_{2j}, p_{2k}]}_{i\hbar\delta_{jk}}\Big) = i\hbar \quad \checkmark$$

$$[R_j, P_k] = \left[\frac{m_1 r_{1j} + m_2 r_{2j}}{m_1+m_2}, p_{1k} + p_{2k}\right]$$

As before: $[r_{1j}, p_{2k}] = 0$

$$= \frac{1}{m_1+m_2}\left(m_1 \underbrace{[r_{1j}, p_{1k}]}_{i\hbar\delta_{jk}} + m_2 \underbrace{[r_{2j}, p_{2k}]}_{i\hbar\delta_{jk}} \right) = i\hbar\delta_{jk}$$

So the CM and relative operators obey the usual position-momentum commutation relations. I guess to be really careful we should verify $[r_j, P_k] = \phi = [R_j, p_k]$

$$[r_j, P_k] = [r_{1j} - r_{2j}, p_{1k} + p_{2k}] = [r_{1j}, p_{1k}] - [r_{2j}, p_{2k}]$$

$$= i\hbar\delta_{jk} - i\hbar\delta_{jk} = 0$$

I leave $[R_j, p_k]$ to you.

The proof that $p_1^2/2m_1 + p_2^2/2m_2 = p^2/2\mu + P^2/2M$ for QM follows the same algebra that we made when we considered classical mechanics.

So the final thing to point out is the analogy of the classical observation that the eqns of motion for $(\underset{\sim}{r}, p)$ decouple from those of $(\underline{R}, \underline{P})$.

to see this, write $\psi(R, \underset{\sim}{r}) = \Phi(R)\phi(r)$

$$\left[\frac{\underline{P}^2}{2M} + \frac{p^2}{2\mu} + V(r) \right] \psi(R, r) = E' \psi(R, r)$$

is satisfied by

$$* \qquad \underline{P}^2/2\underline{M} \; \Phi(R) = E \, \Phi(R)$$

with $E' = E + \epsilon$

$$\left(p^2/2\mu + V(r) \right) \phi(r) = \epsilon \phi(r)$$

ie two <u>independent</u> Schroedinger eqns.

The analog of the classical $\dot{\underline{P}} = 0$ is that the solution of $*$ is

$$\Phi(R) = e^{i \underline{K} \cdot \underline{R}} \quad \text{with} \quad E = \hbar^2 K^2 / 2\underline{M}$$