Problem Set 5

Instructions:

1. Answer all questions below. Show your work for full credit.
2. Read partial derivative symbols, e.g., $\partial/\partial x$, as d/dx if you are unfamiliar.
3. The first problem is due at the start of class on 14 Oct 2013
4. The second problem is due at the start of class on 16 Oct 2013
5. The remaining problems are due by the end of the day on 18 Oct 2013
6. You may collaborate, but everyone must turn in their own work.

Daily problem for 14 Oct

(a) Show that the speed of an electron in the nth Bohr orbit of hydrogen is $\alpha c/n$, where α is the fine structure constant, equal to $e^2/4\pi\epsilon_o\hbar c \approx 1/137$.

(b) What would be the speed in a hydrogen-like atom with a nuclear charge of Ze?

(c) Let's say our threshold for worrying about relativistic effects when it amounts to a 10% correction, where $\gamma = 1.10$ (implying $v/c \approx 0.42$). For the ground state of a hydrogen-like atom, for which element do we reach this threshold?

(d) Following the previous question, at what element is the correction 50% ($\gamma = 1.5$, $v/c \approx 0.745$).[i]

Daily problem for 16 Oct The wave function for a particle is given by

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad \{A, B\} \in \mathbb{R} \tag{1}$$

Identifying $|\psi(x)|^2$ as a 'probability density,' the quantum-mechanical analog of current density is[ii]

$$j(x) = \frac{\hbar}{2mi}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right) \tag{2}$$

(a) What current does the wave function above represent? *Be careful with signs and complex conjugates.*

(b) What is the physical interpretation of your result (hint: the wave function is the sum of right- and left-traveling waves).

(c) For a bound-state wave function (a wave that isn't traveling), ψ can be chosen to be purely real, and $\psi^* = \psi$. What does this indicate about the current density for bound states?

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[i] The inclusion of relativistic effects on electron orbitals has dramatic consequences for heavier elements like Hg: `http://www.rsc.org/chemistryworld/2013/06/why-mercury-liquid-relativity-evidence`

[ii] The current density may be regarded as a 'probability current' whose integral over a closed surface is equal to the rate of change of the probability that the particle will be found inside this surface. You may also note that $\frac{\hbar}{mi}\frac{\partial}{\partial x}$ is just the operator for the velocity of the particle (compare it to the momentum operator).

The remaining problems are due 18 Oct 2013

1. In electromagnetic theory, the conservation of charge is represented by the continuity equation (in one dimension)

$$\frac{\partial j}{\partial x} = -\frac{\partial \rho}{\partial t} \tag{3}$$

Make use of the quantum-mechanical probability current density given in the preceding problem.

- **(a)** Show that the continuity equation above is satisfied with the quantum definition of current density and probability density $\rho = |\psi|^2$. *Be careful with signs and complex conjugates, and note problem 5 part iii.*
- **(b)** For a plane wave $\psi = Ae^{i(kx-\omega t)}$, show that probability current can be written $|A|^2 v = \rho v$, where v is the particle's velocity .
- **(c)** For the same plane wave, show that the probability density has no explicit time dependence. This illustrates that the particle may be moving (nonzero current) even though the probability density isn't changing in time.

2. An electron is in the $n=5$ state of hydrogen. To what states can the electron make transitions, and what are the energies of the emitted electrons?

3. Find the directions in space where the angular probability density for the $l=2$, $m_l=0$ electron in hydrogen has its maxima and minima.

4. What is the probability of finding an $n=2$, $l=1$ electron between a_o and $2a_o$?

5. *Links between quantum and classical physics.* In classical mechanics, from the definition of momentum, we can put $dx/dt = p_x/m$. In quantum mechanics, this is replaced by a corresponding relation between expectation values:

$$\frac{d}{dt}\langle x\rangle = \frac{\langle p_x\rangle}{m} \tag{4}$$

Verify this result with the help of the following outline:

- **(i)** Take the basic definition

$$\langle x\rangle = \int\limits_{\text{all } x} \psi^*(x,t)x\psi(x,t)\,dx \tag{5}$$

We do not need to specify the precise form of ψ.

- **(ii)** Taking the time derivative, we find

$$\frac{d}{dt}\langle x\rangle = \int\limits_{\text{all } x} \frac{\partial \psi^*}{\partial t}x\psi\,dx + \int\limits_{\text{all } x} \psi^* x\frac{\partial \psi}{\partial t}\,dx \tag{6}$$

(On the right, x is just the variable of integration, and is not subject to the d/dt operation.)

(iii) Replace $\partial\psi/\partial t$ and $\partial\psi^*/\partial t$ by using the time-independent Schrödinger equation and its counterpart for ψ^*:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}+V(x)\psi^*=-i\hbar\frac{\partial\psi^*}{\partial t} \tag{7}$$

(iv) Carry out the integrations over all x, taking advantage of the fact that ψ vanishes for $x\to\pm\infty$ (integration by parts is involved).

(v) Use the relationship $p_{\mathrm{op}}\psi=\frac{\hbar}{i}\frac{\partial\psi}{\partial x}$

6. Referring to the preceding question, see if by means of a similar approach you can obtain the quantum-mechanical counterpart of Newton's second law:

$$\frac{d}{dt}\langle p_x\rangle=\langle F_x\rangle=\langle -\frac{\partial V}{\partial x}\rangle \tag{8}$$

7. Find the most probable radius **and** the expected value of the radial position $\langle r\rangle$ of an electron in the $2p$ state.

$$\psi_{2p}=\frac{1}{\sqrt{3}\,(2a_o)^{3/2}}\frac{r}{a_o}e^{-r/2a_o} \tag{9}$$

where $a_0=\frac{4\pi\epsilon_0\hbar^2}{m_e e^2}=0.529\times10^{-10}$ m is the Bohr radius.