Massachusetts Institute of Technology
Physics Department

Physics 8.321 — **Fall 2006**
Quantum Theory I — **October 2, 2006**
Assignment 5

Due October 13, 2006

Announcements

- The 8.321 midterm exam will take place in class on October 31 (Hallowe'en). It will be an hour and a half exam.

Reading topics for this period

- Classical mechanics and canonical quantization; Schrödinger and Heisenberg "pictures" of time evolution; two state systems; simple harmonic oscillator.

Reading Recommendations 5

- 8.321 lecture notes on time evolution in quantum mechanics (posted on the website), classical Hamiltonian mechanics, and canonical quantization.
- Sakurai, §2.1 and 2.2 discussed the basics of time evolution including "pictures".
- Review of classical mechanics (in addition to 8.321 posted lecture notes): Shankar, §, especially §2.5-2.7.
- The basics of motion in a magnetic field are presented in Gottfried & Yan, §4.3, which has been scanned and put on the 8.321 website.
- Two state systems are presented in Gottfried & Yan, §4.1, which has been scanned and put on the 8.321 website.
- The harmonic oscillator is discussed in almost every textbook. Sakurai §2.7; Shankar §7; and Gottfried & Yan §4.2.

Problem Set 5

Topics covered in the problems

- Motion of a charged particle in a magnetic field, and the importance of the vector potential in quantum mechanics.

- Motion in the Schrödinger and Heisenberg pictures.
- Time dependence of the density matrix.

1. **Canonical Quantization in the Presence of Static Magnetic and Electric Fields**

   This is an important subject that we will return to from time to time in 8.321 and 8.322. It also illustrates the power as well as the shortcomings of the canonical quantization method. You may have studied the Hamiltonian formulation of this motion in classical mechanics. In that case the first few sections of the problem are review.

   The classical equation of motion for a particle in constant electric and magnetic fields is the Lorentz force law,

   $$m\frac{d^2\vec{x}}{dt^2} = \vec{F} = e\vec{E} + \frac{e}{c}\dot{\vec{x}} \times \vec{B}$$

   (using Gaussian units). Remember that static fields can be described by ϕ and $\vec{A}$, the electrostatic and magnetic vector potentials,

   $$\vec{E} = -\vec{\nabla}\phi \quad \text{and} \quad \vec{B} = \vec{\nabla} \times \vec{A}$$

   (a) Consider the Lagrangian

   $$\mathcal{L} = \frac{1}{2}m\dot{\vec{x}}^2 + \frac{e}{c}\dot{\vec{x}} \cdot \vec{A}(\vec{x}) - e\phi(\vec{x}) \tag{1}$$

   What is the canonical momentum, $\vec{p} = \partial\mathcal{L}/\partial\dot{\vec{x}}$? Note that it is *not* $m\dot{\vec{x}}$. Show that the Euler Lagrange equations, $d\vec{p}/dt = \partial\mathcal{L}/\partial\vec{x}$, give the Lorentz force law. You will have to remember that, although both $\vec{A}$ and ϕ have no explicit time dependence, they depend implicitly on time via the argument $\vec{x}(t)$. Thus $\frac{d}{dt}\vec{A} = (\dot{\vec{x}} \cdot \vec{\nabla})\vec{A}$. [You'll also need some vector calculus identities, or the help of a text like Jackson's.]

   (b) Find the Hamiltonian, $H = \dot{\vec{x}} \cdot \vec{p} - \mathcal{L}$. Combining the results of parts (a) and (b), it appears that the energy can be written as $E = \frac{1}{2}m\dot{\vec{x}}^2 + e\phi$ (an elementary result since the magnetic field does no work). What is the conceptual difference between H and E in classical mechanics?

   (c) Quantize this system canonically: $[x_j, p_k] = i\hbar\delta_{jk}$, *etc.*. Then write the Schrödinger equation in coordinate space.

   (d) Show that $\vec{A} = -\frac{1}{2}\vec{x} \times \vec{B}_0$ is a vector potential corresponding to a constant field $\vec{B}_0$. Substitute this into the Schrödinger equation (with $\phi = 0$) to obtain

   $$\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 - \frac{e}{2mc}\vec{L} \cdot \vec{B}_0 + \frac{e^2}{8mc^2}\rho^2 B_0^2\right)\psi(\vec{x}) = E\psi(\vec{x}) \tag{2}$$

   Here $\vec{L} = \vec{x} \times \vec{p}$ and $\rho = \hat{B}_0 \times \vec{x}$ is the radial coordinate in the plane perpendicular to $\vec{B}_0$.

Show that the magnetic moment of a charge e in an orbit with angular momentum $\vec{L}$ is $\mu = e\vec{L}/2mc$. ($e\hbar/2mc$ is the "Bohr magneton") so the second term in eq. (2) is the interaction of the magnetic field with the dipole moment of the orbiting particle. [If you are unfamiliar with Gaussian units, you can find the expression for the magnetic moment in Jackson's book, for example.]

(e) Choose a coordinate system so $\vec{B}_0$ lies along the $\hat{z}$ direction. Remember from undergraduate quantum mechanics that p_z and L_z commute with $\vec{\nabla}^2$, so the energy eigenstates can be labeled by the eigenvalue of p_z ($\hbar k$) and eigenvalue of L_z ($M\hbar$).

Show that the Schrödinger equation for a particle in a magnetic field reduces to a two dimensional harmonic oscillator with an energy offset due to M and k. What are the energy eigenvalues?[1]

(f) Eq. (2) turns out not to be correct for an electron. The electron has another contribution to its magnetic moment for which there is no classical analogue. The contribution is proportional to its internal spin, $\vec{S} = \frac{1}{2}\hbar\vec{\sigma}$, a quantum variable with no classical analog. Rewrite eq. (2) allowing for a contribution to the magnetic moment proportional to $\vec{S}$. The constant of proportionality, usually denoted g, is called the gyromagnetic ratio. For the electron g is very close to 2. Assume $g = 2$. How does this affect the energies eigenvalues you found in the previous part?

2. **Time Evolution** (Sakurai, §2, Problem 23)

A particle of mass m in one dimension is bound to a fixed center by an attractive δ-function potential, $V(x) = -\lambda\delta(x)$ ($\lambda > 0$). At $t = 0$ the potential is suddenly switched off (that is $V = 0$ for $t > 0$). What is the energy of the particle when $t > 0$? Find the wavefunction for $t > 0$ (be quantitative, but you may not be able to evaluate an integral that appears).

3. **Schrödinger versus Heisenberg**

Consider a free particle moving in one dimension. The Hamiltonian is $H = P^2/2m$.

(a) What are $X_H(t)$ and $P_H(t)$? (where the subscript H means "in the Heisenberg picture".)

(b) What is $[X_H(t), X_H(0)]$?

(c) Suppose the uncertainty in X_H is measured in a certain state at $t = 0$. Call it $\Delta X_H^2(0)$. What does the uncertainty relation tell you about $\Delta X_H^2(t)$?

(d) Consider the *correlation function*

$$C(t) = \langle\psi|X_H(t)X_0(0)|\psi\rangle$$

which arises when we study time dependent processes like the scattering of light. Write an expression for $C(t)$ in the Schrödinger picture. Evaluate $C(t)$ in the harmonic oscillator ground state.

[1] This result is even simpler than it looks because $M = n_1 - n_2$, where n_1 and n_2 are the usual number of "oscillator quanta" in the x and y directions.

4. **Time Dependence of the Density Matrix**

In lecture we discussed only the time dependence of pure states. Mixed states evolve in time too. We defined an arbitrary density matrix by $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$.

(a) The time dependence of states in the Schrödinger picture induces a natural definition of the time dependent density matrix in the Schrödinger picture, $\rho_S(t)$. What is it? Write $\rho_S(t)$ in terms of $\rho_S(0)$ and the time evolution operator $U(t, 0)$. Compare this result with the relation between a Heisenberg picture operator, $Q_H(t)$ and the Schrödinger picture operator, Q_S.

(b) How does the expectation value of an observable, Q, in the mixed state evolve with time? Remember at a fixed time we found $\langle Q\rangle = \mathrm{Tr}[Q\rho]$. What is the analagous equation at a time t, in terms of $\rho_S(t)$, or in terms of $Q_H(t)$?

(c) What is the Schrödinger equation for $\rho_S(t)$?

(d) Prove that a pure state cannot evolve into a mixed state or vica versa.

5. **Quantum Consequences of a Magnetic Field** (Sakurai, §2, Problem 25)

Consider an electron confined to the *interior* of a hollow cylindrical shell whose axis coincides with the z-axis. The wave function is required to vanish on the inner and outer walls, $\rho = \rho_a$ and $\rho = \rho_b$, and also at the top and bottom, $z = 0, L$.

(a) Find the energy eigenvalues and eigenfunctions (ignore normalization). Show that the eigenvalues are given by

$$E_{lmn} = \frac{\hbar^2}{2m_e}\left(k_{mn}^2 + \left(\frac{l\pi}{L}\right)^2\right)$$

where k_{mn} is the n^{th} root of the transcendental equation,

$$J_m(k_{mn}\rho_b)N_m(k_{mn}\rho_a) - J_m(k_{mn}\rho_a)N_m(k_{mn}\rho_b) = 0$$

(b) Repeat the same problem when there is a uniform magnetic field, $\vec{B} = B\hat{z}$ for $0 < \rho < \rho_a$. Note that the energy eigenvalues are influenced by the magnetic field even though the electron never "touches" the magnetic field.

(c) Compare, in particular, the ground state of the $B = 0$ problem with that of the $B \neq 0$ problem. Show that if we require the ground state energy to be unchanged in the presence of B, we obtain the "flux quantization" condition,

$$\pi\rho_a^2 B = \frac{2\pi N\hbar c}{e}, \quad \text{for} \quad N = 0, \pm 1, \pm 2, \pm 3, ...$$