Physics 195a
Problem set number 5 – Solutions to Problems 24 and 29
Due 2 PM, Thursday, November 7, 2002

Notes about course:

- Homework should be turned in to the TA's mail slot on the first floor of East Bridge.
- Collaboration policy: OK to work together in small groups, and to help with each other's understanding. Best to first give problems a good try by yourself. Don't just copy someone else's work – whatever you turn in should be what you think you understand.
- There is a web page for this course, which should be referred to for the most up-to-date information. The URL:
  http://www.hep.caltech.edu/~fcp/ph195/
- TA: Anura Abeyesinghe, anura@caltech.edu
- If you think a problem is completely trivial (and hence a waste of your time), you don't have to do it. Just write "trivial" where your solution would go, and you will get credit for it. Of course, this means you are volunteering to help the rest of the class understand it, if they don't find it so simple...

READING: Read the "The K^0: An Interesting Example of a 'Two-State' System" course note.

PROBLEMS:

24. Suppose we have a system with total angular momentum 1. Pick a basis corresponding to the three eigenvectors of the z-component of angular momentum, J_z, with eigenvalues $+1, 0, -1$, respectively. We are given an ensemble described by density matrix:

$$\rho = \frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}.$$

(a) Is ρ a permissible density matrix? Give your reasoning. For the remainder of this problem, assume that it is permissible. Does it describe a pure or mixed state? Give your reasoning.

Solution: Clearly ρ is hermitian. It is also trace one. This is almost sufficient for ρ to be a valid density matrix. We can see this by noting that, given a hermitian matrix, we can make a transformation of basis to one in which ρ is diagonal. Such a transformation preserves the trace. In this diagonal basis, ρ is of the form:

$$\rho = a|e_1\rangle\langle e_1| + b|e_2\rangle\langle e_2| + c|e_3\rangle\langle e_3|,$$

where a, b, c are real numbers such that $a + b + c = 1$. This is clearly in the form of a density operator. Another way of arguing this is to consider the n-term dyad representation for a hermitian matrix.

However, we must also have that ρ is positive, in the sense that a, b, c cannot be negative. Otherwise, we would interpret some probabilities as negative. There are various ways to check this. For example, we can check that the expectation value of ρ with respect to any state is not negative. Thus, let an arbitrary state be: $|\psi\rangle = (\alpha, \beta, \gamma)$. Then

$$\langle\psi|\rho|\psi\rangle = 2|\alpha|^2 + |\beta|^2 + |\gamma|^2 + 2\Re(\alpha^*\beta) + 2\Re(\alpha^*\gamma). \tag{10}$$

This quantity can never be negative, by virtue of the relation:

$$|x|^2 + |y|^2 + 2\Re(x^*y) = |x + y|^2 \geq 0. \tag{11}$$

Therefore ρ is a valid density operator.

To determine whether ρ is a pure or mixed state, we consider:

$$\mathrm{Tr}(\rho^2) = \frac{1}{16}(6 + 2 + 2) = \frac{5}{8}.$$

This is not equal to one, so ρ is a mixed state. Alternatively, one can show explicitly that $\rho^2 \neq \rho$.

(b) Given the ensemble described by ρ, what is the average value of J_z?

Solution: We are working in a diagonal basis for J_z:

$$J_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The average value of J_z is:

$$\langle J_z \rangle = \mathrm{Tr}(\rho J_z) = \frac{1}{4}(2 + 0 - 1) = \frac{1}{4}.$$

(c) What is the spread (standard deviation) in measured values of J_z?
Answer: We'll need the average value of J_z^2 for this:

$$\langle J_z^2 \rangle = \mathrm{Tr}(\rho J_z^2) = \frac{1}{4}(2 + 0 + 1) = \frac{3}{4}.$$

Then:

$$\Delta J_z = \sqrt{\langle J_z^2 \rangle - \langle J_z \rangle^2} = \frac{\sqrt{11}}{4}.$$

25. Coherent states with density matrices: Exercise 7 of the "Density Matrix Formalism" course note.

26. Density matrix for a spin 1/2 system in a magnetic field: Exercise 8 of the "Density Matrix Formalism" course note.

27. Entropy for a system of spin 1/2 particles in a magnetic field: Exercise 9 of the "Density Matrix Formalism" course note.

28. Hamiltonian in the particle-antiparticle basis: Exercise 1 of the K^0 course note.

29. Review of Schrödinger equation in three dimensions: Central potential problem. There are some areas of elementary quantum mechanics that I want to make sure don't fall through the cracks in your education, in particular, the central force problem and the specific case of the one-electron atom.

    Suppose we have two particles, of masses m_1 and m_2, described by position coordinates $\mathbf{x}_1$ and $\mathbf{x_2}$. Assume that they interact with each other via a potential $V(\mathbf{x}_1, \mathbf{x}_2)$.

(a) Write down the Hamiltonian for this system. Show that it may be transformed to a description in terms of center-of-mass and relative coordinates. Show that the problem then reduces to two problems: one for the center-of-mass motion, and one for the relative motion, if the potential can be separated into a term depending only on the position of the center-of-mass, plus a term depending only on the relative locations of the particles. Now assume that the potential does not depend on the center-of-mass position, and solve for the center-of-mass motion. Is your solution sensible?

Solution: Let $\mathbf{p}_i = -i\nabla_i$ denote the momentum of particle i, with magnitude p_i. The Hamiltonian is:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(\mathbf{x}_1, \mathbf{x}_2) = -\frac{\nabla_1^2}{2m_1} - \frac{\nabla_2^2}{2m_2} + V(\mathbf{x}_1, \mathbf{x}_2) \quad (12)$$

Define total mass and center-of-mass position and momentum variables:

$$\begin{aligned} M &= m_1 + m_2 && (13)\\ \mathbf{X} &= \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{M} && (14)\\ \mathbf{P} &= M\dot{\mathbf{X}} = \mathbf{p}_1 + \mathbf{p}_2. && (15) \end{aligned}$$

Define the reduced mass and relative position and momentum variables:

$$\begin{aligned} m &= \frac{m_1 m_2}{m_1 + m_2} && (16)\\ \mathbf{x} &= \mathbf{x}_1 - \mathbf{x}_2 && (17)\\ \mathbf{p} &= m\dot{\mathbf{x}} = \frac{m_2\mathbf{p}_1 - m_1\mathbf{p}_2}{M}. && (18) \end{aligned}$$

We may solve for $\mathbf{x}_1$ and $\mathbf{x}_2$ in terms of $\mathbf{X}$ and $\mathbf{x}$:

$$\begin{aligned} \mathbf{x}_1 &= \mathbf{X} + \frac{m_2}{M}\mathbf{x} && (19)\\ \mathbf{x}_2 &= \mathbf{X} - \frac{m_1}{M}\mathbf{x} && (20)\\ & && (21) \end{aligned}$$

Then the Hamiltonian can be written in terms of center-of-mass and relative coordinates according to (letting $P = |\mathbf{P}|$ and $p = |\mathbf{p}|$):

$$H = \frac{P^2}{2M} + \frac{p^2}{2m} + V(\mathbf{X} + \frac{m_2}{M}\mathbf{x}, \mathbf{X} - \frac{m_1}{M}\mathbf{x}) \tag{22}$$

Now let $U_T(\mathbf{X}, \mathbf{x}) = V(\mathbf{X} + \frac{m_2}{M}\mathbf{x}, \mathbf{X} - \frac{m_1}{M}\mathbf{x})$, and assume that it is of the form:

$$U_T(\mathbf{X}, \mathbf{x}) = U_{CM}(\mathbf{X}) + U(\mathbf{x}). \tag{23}$$

Let ∇_{CM} be the gradient operator with respect to $\mathbf{X}$, and ∇ be the gradient with respect to $\mathbf{x}$. Then we may write the Schrödinger equation as:

$$\left[-\frac{\nabla_{CM}^2}{2M} - \frac{\nabla^2}{2m} + U_{CM}(\mathbf{X}) + U(\mathbf{x})\right]\psi(\mathbf{X}, \mathbf{x}) = E\psi(\mathbf{X}, \mathbf{x}). \tag{24}$$

We expand ψ in a series of terms of the form $\Phi(\mathbf{X})\phi(\mathbf{x})$, and apply the technique of separation of variables to obtain:

$$\frac{1}{\Phi}\left[-\frac{\nabla_{CM}^2}{2M} + U_{CM}(\mathbf{X})\right]\Phi = E_{CM} \tag{25}$$

$$\frac{1}{\phi}\left[-\frac{\nabla^2}{2M} + U(\mathbf{x})\right]\phi = E - E_{CM} \tag{26}$$

Now we assume $U_{CM}(\mathbf{X}) = 0$. We may solve for the center-of-mass motion:

$$-\frac{\nabla_{CM}^2}{2M}\Phi(\mathbf{X}) = E_{CM}\Phi(\mathbf{X}) \tag{27}$$

The solution is

$$\Phi(\mathbf{X}) = Ae^{i\mathbf{P}\cdot\mathbf{x}} + Be^{-i\mathbf{P}\cdot\mathbf{x}}, \tag{28}$$

with $E_{CM} = \frac{P^2}{2M}$. This is simply the motion of a free particle of mass M.

(b) Suppose V is a function of the separation between the two particles only, $V = V(|\mathbf{x}|)$, where $\mathbf{x} \equiv \mathbf{x}_1 - \mathbf{x}_2$. Solve the Schrödinger equation for the angular dependence and show that the Schrödinger equation may be reduced to an equivalent one dimensional problem. Give the "effective potential" for this equivalent one dimensional problem.

Solution: We have the Schrödinger equation for the relative motion (letting $|\mathbf{x}| \equiv r$):

$$\left[-\frac{\nabla^2}{2m} + V(r)\right]\psi(\mathbf{x}) = E\psi(\mathbf{x}). \tag{29}$$

Since the problem clearly has spherical symmetry, we adopt spherical polar coordinates. The Laplacian in spherical polar coordinates is:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta)}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{(r\sin\theta)^2}\frac{\partial^2}{\partial\phi^2}. \tag{30}$$

Once again we use the method of separation of variables. The solution to the angular portion is $Y_{\ell m}(\theta,\phi)$:

$$\left[-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta)}\sin\theta\frac{\partial}{\partial\theta} - \frac{1}{(\sin\theta)^2}\frac{\partial^2}{\partial\phi^2}\right]Y_{\ell m}(\theta,\phi) = \ell(\ell+1)Y_{\ell m}(\theta,\phi) \tag{31}$$

The remaining dependence is on r. Letting $\psi(\mathbf{x}) = R(r)Y_{\ell m}(\theta,\phi)$, we have:

$$\left[-\frac{1}{2mr^2}\frac{d}{dr}r^2\frac{d}{dr} + V(r) + \frac{\ell(\ell+1)}{2mr^2}\right]R(r) = ER(r). \tag{32}$$

Write $R(r) = u(r)/r$ to obtain:

$$\left[-\frac{1}{2m}\frac{d^2}{dr^2} + V(r) + \frac{\ell(\ell+1)}{2mr^2}\right]u(r) = Eu(r). \tag{33}$$

Thus, we have reduced our problem to one of solving a one-dimensional Schrödinger equation, with an "effective potential" $V(r) + \frac{\ell(\ell+1)}{2mr^2}$. The $\ell(\ell+1)$ term may be interpreted as a "centrifugal barrier" due to angular motion.