Physics 401 - Homework #8

1) **Three-state system (three points each).** Suppose that we have a physical system for which there are only three states. For example, perhaps the system is a molecule where the atoms can take on three different arrangements. Regardless of how we interpret the physical meaning of the three states, we can write down the equations of quantum mechanics for this system using these states as a basis. As usual, we will assume that the states are orthonormal and complete. In other words, let's assume that any state can be thought of as a superposition of the three base states, and that different states have no overlap.

Let's further suppose that the Hamiltonian for this system in our three-state basis is:

$$\hat{H} = \begin{pmatrix} E_0 & -A & 0 \\ -A & E_0 & 0 \\ 0 & 0 & E_3 \end{pmatrix}$$

Then the time-independent Schroedinger Equation is:

$$\begin{pmatrix} E_0 & -A & 0 \\ -A & E_0 & 0 \\ 0 & 0 & E_3 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = E_n \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

a) Find the three energy eigenvectors and energy eigenvalues (E_n) for this system. To answer this question, you may either use the methods of linear algebra, or you may guess the eigenvectors, show that your guesses are correct, and find the eigenvalues through direct substitution. (By the way, it's a good habit to always plug your eigenvectors back into the original equation to check your work.)

b) Write down the fully time-dependent solutions for the three stationary states of this system. In other words, show how each eigenvector found in part (a) evolves in time.

c) We have not specified the physical meaning of our three base states, but there is one question that we can answer about them. Are our base states the energy eigenstates?

d) Sometimes people use Dirac notation to write down a Hamiltonian. If we label our three states as (1), (2), and (3), then the Hamiltonian can be written as

$$\hat{H} = E_0\left(|1\rangle\langle 1| + |2\rangle\langle 2|\right) - A\left(|1\rangle\langle 2| + |2\rangle\langle 1|\right) + E_3|3\rangle\langle 3|$$

Using this Dirac-notation operator, calculate the nine matrix elements of the Hamiltonian, and show that the result is the same as the Hamiltonian matrix written above. Remember,

the matrix elements of the Hamiltonian are given by $H_{ij} = \langle i | \hat{H} | j \rangle$, where $\{ | j \rangle \}$ are the base states that we have chosen to use.

2) **The particle-in-the-box and the harmonic oscillator in the energy basis (three points each).** We already know the energy eigenvalues for the particle-in-the-box and the harmonic oscillator. So we can quickly write down the Hamiltonians for these systems in the energy basis. (Remember: in the energy basis, the Hamiltonian is a diagonal matrix.)

a) Write down the Hamiltonian matrix for the particle-in-the-box in the energy basis. (Note: since this basis has an infinite number of states, the Hamiltonian matrix is a square matrix with an infinite number of columns and rows. Obviously, you should only write down a small corner of the matrix, like the three-by-three upper left-hand corner. Then you can make liberal use of the ellipsis (...) to show how the matrix continues.)

b) Write down the Hamiltonian matrix for the harmonic oscillator.

c) The promotion and demotion operators for the harmonic oscillator have the following simple effect on the energy eigenstates:

$$\hat{a} | n \rangle = \sqrt{n} | n-1 \rangle, \quad \hat{a}^t | n \rangle = \sqrt{n+1} | n+1 \rangle$$

Use these expressions to calculate the matrix elements for both of these operators in the energy basis. Remember, the matrix elements are given by $a_{mn} = \langle m | \hat{a} | n \rangle$ and $a^t_{mn} = \langle m | \hat{a}^t | n \rangle$.

d) Use your result from part (c) to write the promotion and demotion operators explicitly in matrix notation. In other words, I want you to write down the matrix elements for the promotion and demotion operators as a bunch of rows and columns with a big set of parentheses around them.

e) (three points) The number operator is defined by $\hat{N} \equiv \hat{a}^t \hat{a}$. Multiply together your matrices for the promotion and demotion operators to calculate the matrix which represents the number operator. Is your Hamiltonian matrix related to the number operator matrix according to $\hat{H} = \hbar \omega_0 \left(\hat{N} + \frac{1}{2} \right)$? Answer: it should be!

Here's why matrix multiplication gives the right result for the number operator. We can calculate the matrix elements of the number operator like this:

$$N_{mn} \equiv \langle m|\hat{N}|n\rangle = \langle m|\hat{a}^t\hat{a}|n\rangle = \langle m|\hat{a}^t\left(\sum_l |l\rangle\langle l|\right)\hat{a}|n\rangle = \sum_l \langle m|\hat{a}^t|l\rangle\langle l|\hat{a}|n\rangle = \sum_l a^t_{ml}a_{ln}$$

$$\therefore N_{mn} = \sum_l a^t_{ml}a_{ln}$$

In this calculation, we've inserted the identity operator between the promotion and demotion operators. In our identity operator, the sum is over energy eigenstates, which we've labeled using the subscript (l).

The last expression is simply the rule for matrix multiplication, so we conclude that multiplying the matrices for the promotion and demotion operators gives the correct matrix for the number operator.

f) Using your matrix representations of the promotion and demotion operators in the energy basis, write down the matrices which represent the position and momentum operators in the energy basis.

Here's the bottom line. In Schroedinger wave mechanics, we think of quantum mechanical systems in terms of the wave functions Ψ(x,t) and/or Φ(k,t). These wavefunctions are a continuum of probability amplitudes. Since position and momentum are continuous, the operators in wave mechanics are differential operators, and the equation of motion is a partial differential equation.

In Heisenberg's matrix mechanics, we think in terms of discrete states, like the energy eigenstates of bound systems. Then the quantum state of the system is represented by a column vector, the operators are matrices, and the equation of motion is a matrix equation. We see that even familiar operators like the momentum and position operators can be viewed as matrices from the point of view of a discrete basis.

3) **An operator in an exponent.** We can define functions of operators in much the same way that we define functions of ordinary variables. In quantum mechanics we often have reason to create an operator by putting some other operator in an exponent.
For example, if we put the Hamiltonian operator in an exponent like this:

$$\hat{U}(t) \equiv \exp\left(\frac{-it\hat{H}}{\hbar}\right)$$

we get an operator which we call the "time-evolution operator".

a) In order to make any sense of the time-evolution operator, we first have to define what we mean by putting an operator into an exponent. We define the meaning of this expression by the Taylor series for the exponential function. Write down the first few terms of this series for the time evolution operator.

b) Using wave mechanics notation, write down our old, familiar expression for the arbitrary initial state wavefunction in the position basis ($\Psi(x,t=0) = \psi(x)$) as an expansion in terms of energy eigenfunctions in the position basis.

c) Show that when you apply the Taylor series definition of the time-evolution operator to the initial state wavefunction, the result is the fully time-dependent wavefunction $\Psi(x,t)$. In other words, show that

$$\Psi(x,t) = \hat{U}(t)\Psi(x,t=0)$$

So the time-evolution operator is another way to specify how quantum mechanical states evolve in time. It is completely equivalent to the Schroedinger equation.