Physics 401 - Homework #9 - Due Wednesday November 18th

1) The time evolution operator in matrix mechanics. In Homework #8, we showed that the time-evolution operator takes an initial state wavefunction and "translates it in time" as described by the Schrödinger equation. In this problem we will demonstrate a similar result for the matrix mechanics version of the time-evolution operator.

a) (three points) In some arbitrary discrete basis, our state vector is a set of QM amplitudes \( \{C_i(t)\} \). Using matrix element notation, a small displacement in time can be written

\[
C_i(t = \Delta t) = \sum_j U_{ij}(\Delta t)C_j(t = 0)
\]

where \( U_{ij}(\Delta t) \) is the matrix element of the time evolution operator. Use the Taylor series definition of the time evolution operator to calculate \( U_{ij}(\Delta t) \) for a small time increment. You may approximate by keeping only the zeroth-order and first-order terms in the Taylor series, and your result should be a sum of the identity matrix element \( \delta_{ij} \) (the Kronecker delta) and a second term which is proportional to \( \Delta t \).

b) (three points) The equation from part (a) says that we should multiply the \( U \) matrix by the column vector \( C \), and it's easy to do this multiplication for the Kronecker delta part of the \( U \) matrix. Go ahead and do that multiplication by summing over \( (j) \) for that term.

c) (three points) Move the right-hand side term which you summed in part (b) to the left-hand side of the equation, and divide the equation by \( \Delta t \). Take the limit as \( \Delta t \) goes to zero, and your result should be the matrix mechanics form of the Schrödinger equation. This demonstrates once again that the time-evolution operator is equivalent to the Schrödinger equation.

2) The position displacement operator (three points). Because of the role that the Hamiltonian plays in the time evolution operator, we say that "the Hamiltonian generates displacements in time." In a similar fashion, the momentum operator "generates displacements in space". In other words,

\[
e^{i\hbar \hat{p}/\hbar} f(x) = f(x + \Delta x)
\]

Show that this is true, using the familiar form of the momentum operator in position space, and using the Taylor series definition of an operator inside an exponential.

3) A Unitarity-Similarity transformation. In Homework #8, problem #1, we studied a three state system and found its stationary states. In this problem we will do some further calculations for this system. To be more concrete about this system, let's imagine that the basis in which the Hamiltonian was written in Homework #8 is a three-valued position basis, analogous to the up/down basis which we used for the two-state ammonia
molecule. (For example, maybe there is an atom that can be located in three spots in some molecule.)

a) (3 points) Calculate the matrix U which transforms the state vectors in position space into state vectors in the energy basis.

b) (3 points) Confirm that your U matrix is correct by explicitly transforming the energy eigenvectors written in the position basis into the energy basis. (What should the energy eigenvectors look like in the energy basis?)

c) (3 points) Use your U matrix to transform the Hamiltonian from the position basis into the energy basis. This transformation should diagonalize the Hamiltonian matrix, and this diagonalization process is equivalent to finding the energy eigenvectors in position space as you did on Homework #8. For this reason, when someone solves a quantum mechanical problem, they sometimes say that they "diagonalized the Hamiltonian". This terminology is used even when the problem was solved completely in the wave mechanics formalism, without ever writing down a matrix.

4) **Orbital angular momentum operators (three points).** The quantum mechanical operators for orbital angular momentum are defined by analogy with the classical angular momentum:

\[
\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\
\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\
\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x
\]

Using the "canonical commutation relations":

\[ [\hat{x}, \hat{p}_z] = i\hbar \]
\[ [\hat{y}, \hat{p}_x] = i\hbar \]
\[ [\hat{z}, \hat{p}_y] = i\hbar \]

calculate \([\hat{L}_x, \hat{L}_y]\). Hint #1: there is no need to use the explicit form of these operators to answer this question. The canonical commutation relations alone are enough to determine the result. Hint #2: operators for orthogonal directions commute. So, for example, the commutator of \(\hat{x}\) and \(\hat{p}_z\) is zero.