Problem Set 7

Due Tuesday November 26 9:30 AM.
Submit in class or in TA's mailbox in the Physics office.

1. This is meant to be a slightly long but straightforward problem to make sure you are comfortable with time dependence in 2-level systems and with changes of bases. Please make sure you have mastered these concepts.

   Let's consider the ammonia molecule in an electric field. You can use the results from class, and please use the notation from class. Consider the intermediate coupling case where the energy of the dipole in the field $U = -\vec{E} \cdot \vec{d}$ is related to the inter-well coupling energy Δ by $U = \frac{3}{4}\Delta$. For concreteness, let us say that $\vec{E}$ points to the right.

   For this particular ratio of the interaction energies, the coefficients of the eigenstate in the $|1\rangle$, $|2\rangle$ basis are particularly simple expressions in terms of Δ. So, you will have an easier time in this case if you work out the simple algebra directly for the values given, rather than representing the Hamiltonian in terms of mixing angles. Since this is easy, solve the equations on paper without resorting to a computer.

   (a) At $t = 0$ the molecule is prepared to be in its ground-state configuration $|\varphi_g\rangle$. Write an expression describing the probability that, at some time t later, the molecule will be found with the nitrogen atom pointing to the left.

   (b) Related to what you found, argue that the expectation value of any observable (whether or not it commutes with H) will be time-independent, given that initial state.

   (c) Now consider the case that the molecule is oriented with the N atom pointing left at $t = 0$, that is $|\psi(t=0)\rangle = |L\rangle \approx |1\rangle$. Express this initial state in terms of eigenstates of H. Next, write an expression for the time-dependent state $|\psi(t)\rangle$. (Hint: Once you know the coefficients for $t = 0$, adding time dependence should be done instantly without costing you any lines of math, but nobody got this when I asked in class. Make sure you can write down the expression instantly, without thinking about projections etc.)

   (d) For $|\psi(t=0)\rangle = |1\rangle$, find an expression for the probability of finding the system at some time later in the ground energy state $|\varphi_g\rangle$. Argue why there should be no time dependence.

   (e) For $|\psi(t=0)\rangle = |1\rangle$, find an expression for the probability of finding the system at some time later in the state $|1\rangle$. Why is there now a time dependence?

   (f) There is a parity selection rule for absorbing a photon by an electric dipole transition, so checking for absorption of radiation provides a way to measure the parity of the system. Using the following approach, find the expectation value of a parity measurement as a function of time, $\langle \Pi \rangle (t)$, for the initial condition $|\psi(t=0)\rangle = |1\rangle$. First write down a matrix describing the action of the parity-inversion operator Π in the $|1\rangle$, $|2\rangle$ basis. Then use your earlier expression for the energy eigenstates in that basis in order to find the matrix elements of Π in the basis of energy eigenstates. From here, the expectation value can be calculated for the time-evolving state $|\psi(t)\rangle$. Do a check on your answer by verifying that you get the same value for $\langle \Pi \rangle (t = 0)$ using either basis.

(g) Why was parity not conserved? Pick a different relationship between U and Δ which will lead to conservation of parity. Using the same initial state (which is not an eigenstate of parity), verify that $\langle \Pi \rangle$ is time-independent. (Since you have changed the Hamiltonian, the eigenstates states $|\varphi_g\rangle$ and the upper-energy state $|\varphi_u\rangle$ now represent different superpositions of $|1\rangle$ and $|2\rangle$ than they did earlier.)

2. Consider a system of five atomic sites arranged in a square, with site 5 at the center of the square. Let

$$\langle \varphi_i | H | \varphi_{i+1} \rangle = -\Delta, \; i = 1,2,3 \tag{1}$$
$$\langle \varphi_4 | H | \varphi_1 \rangle = -\Delta \tag{2}$$
$$\langle \varphi_i | H | \varphi_5 \rangle = -\Delta, \; i = 1,2,3,4 \tag{3}$$
$$\langle \varphi_i | H | \varphi_i \rangle = \varepsilon, \; i = 1,2,3,4,5 \tag{4}$$
$$\tag{5}$$

where Δ is real. All other matrix elements, apart from those constrained by the fact that H is Hermitian, are 0.

(a) To begin, ignore site 5, and diagonalize the projection of H into the span of $|\varphi_1\rangle$ through $|\varphi_4\rangle$. You can find the eigenvectors by guessing–no need to use a computer.

(b) Try these eigenvectors as eigenvectors of H in the full problem. Show that three of the four are indeed eigenvectors of the full Hamiltonian, with the same eigenvalues.

(c) The remaining two eigenvectors of the full H must be linear combinations of the remaining state from part (a) and the state $|\varphi_5\rangle$. Find these eigenvectors and their associated eigenvalues.

(d) Explain the results of this problem using a symmetry of H, that is, a unitary matrix R that commutes with H.