

Physics 570B, Spring 2011
Assignment 08
Due Tuesday, Mar. 22

Our midterm exam will be on Thursday, March 24. You may bring two pages of hand-written notes to this exam. You may not use calculators, cell phones or other aids during the exam.

1. In the usual basis, the generators of angular momentum for a spin 1/2 object are represented by the matrices:

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1)$$

In some other basis they are represented by

$$S'_x = \frac{\hbar}{2} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad S'_y = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad S'_z = \frac{\hbar}{2} \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \quad (2)$$

First, verify that the second set of matrices satisfies the appropriate commutation relations. Find the unitary transformation that connects one basis to the other, and verify that your answer does what you want. *Hints:* Begin by considering the eigenvectors of L_z . Of course, these are very simple when L_z is diagonal. But this eigenvector is physically the same in both basis sets, so your unitary transformation must map $(1, 0)$ into the eigenvector in the other basis set. After you do this for both eigenvectors, you will have a transformation that works for L_z . Now you need to get L_x and L_y right. Fortunately, you still have the freedom to rotate around the z axis. Equivalently, you have some arbitrary phases in the eigenvectors that you can use.

2. The nuclei of a diatomic molecule are moving in a potential (which includes the nucleon-nucleon interaction and the electronic energy)

$$\epsilon(R) = -2D \left[(a_0/R) - (a_0^2/R^2) \right] \quad (3)$$

Find the vibrational and rotational energies of the molecule.

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Now let's try a couple of highly unphysical but nevertheless educational toy molecules:

3. Consider a one dimensional toy molecule, “delta-onium”. In center-of-mass coordinates for the nuclei, this molecule has two nuclei at $x = a$ and $x = -a$, and one electron. The hamiltonian is $P_{rel}^2/2M_{reduced} + p_e^2/2m - \lambda\delta(x - a) - \lambda\delta(x + a)$. Write the lowest energy bonding and antibonding wave functions for the electron, and find the equation that (implicitly) determines the imaginary wave number (κ) and hence the electronic energy. Draw a graph of this energy as a function of the internuclear separation. What is the binding energy of this molecule?
4. Consider another “cartoon” version of the H_2^+ molecule, where the two nuclei and one electron move in one dimension and interact with harmonic oscillator potentials.

$$\begin{aligned} H &= \frac{P_A^2}{2M} + \frac{P_B^2}{2M} + \frac{P_e^2}{2m} \\ &+ \frac{K_{Ne}}{2} (x_A - x_e)^2 + \frac{K_{Ne}}{2} (x_B - x_e)^2 \\ &- \frac{K_{NN}}{2} (x_A - x_B)^2 \end{aligned} \tag{4}$$

Assume that K_{NN} is small enough that a molecular state exists. In the Born-Oppenheimer approximation compute the effective potential for the vibrational motion of the nuclei, and hence the vibrational energy levels.

HINT: Neither of the last two problems requires a variational approximation.