

# 5.73 Final Exam

You can refer to any book, course notes or research article you like in preparing your solutions to these problems. You may find the following formulae useful:

If  $\mathbf{M} = \begin{pmatrix} E_1 & V \\ V & E_2 \end{pmatrix}$ , and  $E_1 \leq E_2$ , the eigenvalues and eigenvectors of  $\mathbf{M}$  are:

$$E_{\pm} = \frac{E_1 + E_2}{2} \pm \sqrt{\left(\frac{E_1 - E_2}{2}\right)^2 + V^2}$$
$$\mathbf{v}_+ = \begin{pmatrix} \frac{1}{\sqrt{1 + \alpha^2}} \\ \alpha \\ \frac{1}{\sqrt{1 + \alpha^2}} \end{pmatrix} \quad \mathbf{v}_- = \begin{pmatrix} \frac{-\alpha}{\sqrt{1 + \alpha^2}} \\ 1 \\ \frac{1}{\sqrt{1 + \alpha^2}} \end{pmatrix} \quad \alpha \equiv \frac{V}{E_1 - E_2}$$

On this exam, partial credit will be given for incomplete or incorrect solutions, so please briefly summarize how you arrived at your answers.

Problems 1 and 2 are required. You must provide answers to these two problems. You should then pick two of the remaining problems (3,4 and 5) to solve. Please indicate below which of these problems you wish to have graded:

1. (25 pts.) Consider an experiment on a system that can be described using two basis functions. In this experiment, you begin in the ground state of Hamiltonian  $\mathbf{H}_0$  at time  $t_1$ . You have an apparatus that can change the Hamiltonian suddenly from  $\mathbf{H}_0$  to  $\mathbf{H}_1$ . You turn this apparatus on at time  $t_1$ . Then, at time  $t_D > t_1$ , you perform a measurement of an observable,  $D$ . In matrix notation, the Hamiltonians and the operator  $\mathbf{D}$  are given below.

$$\mathbf{H}_0 = \begin{pmatrix} 0 & -4 \\ -4 & 6 \end{pmatrix} \quad \mathbf{H}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix} \quad \mathbf{D} = \begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix}.$$

- a. What are the possible outcomes of the measurement of  $D$ ? What is the state of the system after each measurement?
- b. If you perform many, many measurements, what will be the average observed value of  $D$  as a function of  $t_1$  and  $t_D$ ? Explain the behavior you see.

Problem 1(cont'd)

- c. At  $t_D$ , you measure  $D$ , then the energy and then  $D$  again in rapid (i.e. essentially instantaneous) succession. What is the probability that the two measurements of  $D$  yield the same result?

- d. You perform the experiment, but suspect your apparatus is malfunctioning and turning off at some systematic time  $t_2$  between  $t_1$  and  $t_D$ . In other words, at some time  $t_2$ , you suspect the Hamiltonian is reverting to  $\mathbf{H}_0$ . What qualitative effect would this have on your results from part b.? [Note: this only requires a qualitative description, not a full calculation.]

2. (25 pts.) You had the angular momentum operators for a particular system written down on a scrap of paper. Unfortunately you have misplaced the scrap of paper and you have a meeting with your research advisor in 20 minutes. The only things you remember are that the operators were each represented by 4x4 matrices and that there was one possible value for the total angular momentum. Thus, you have

$$\mathbf{J}_x = \begin{pmatrix} ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \end{pmatrix} \quad \mathbf{J}_y = \begin{pmatrix} ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \end{pmatrix} \quad \mathbf{J}_z = \begin{pmatrix} ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \end{pmatrix}.$$

You are determined to put off your advisor (without lying!) until you find that scrap of paper. Prepare answers to the following potential questions from your advisor. Be as specific as possible.

b. What is  $[\mathbf{J}_x, \mathbf{J}_y]$ ?

c. What is the total angular momentum of the system?

d. What is the matrix representation of  $\mathbf{J}^2 = \mathbf{J}_x^2 + \mathbf{J}_y^2 + \mathbf{J}_z^2$ ?

e. What are the eigenvalues of  $\mathbf{J}_z$ ?

Problem 2 (cont'd)

- f. Denote the eigenvectors of  $\mathbf{J}_z$  by  $\mathbf{c}_m$  where the index  $m$  runs over  $-m_{\max}, -(m_{\max} - 1), \dots, (m_{\max} - 1), m_{\max}$ . Under what conditions can the matrix element  $\mathbf{c}_{m'}^\dagger \cdot \mathbf{J}_x \cdot \mathbf{c}_m$  be non-zero?
- g. Suppose you have two particles, each of which carries an angular momentum described by these matrices. What are the possible eigenvalues of  $\mathbf{J}_{tot}^2 = (\mathbf{J}_1 + \mathbf{J}_2)^2$  and  $\mathbf{J}_z = \mathbf{J}_{1z} + \mathbf{J}_{2z}$ ?

3. (20 pts.) Consider a system that can be described by three basis functions. The full Hamiltonian can be written as  $\hat{H} = \hat{H}_0 + \hat{V}$ . In matrix notation, we have

$$\mathbf{H}_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \mathbf{V} = \begin{pmatrix} \frac{1}{2} & 2 & 0 \\ 2 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

Treat  $\mathbf{V}$  as a perturbation, and determine:

- a. The eigenenergies of the system correct to first order.

- b. The eigenenergies of the system correct to second order.

4. (20 pts.) Consider a system with two diabatic electronic states,  $|1\rangle$  and  $|2\rangle$ , and a single nuclear degree of freedom,  $R$ . The Hamiltonian is given by

$$\hat{H} = |1\rangle\left(-\frac{1}{2}\nabla_R^2 + V_{11}(\hat{R})\right)\langle 1| + |1\rangle V_{12}(\hat{R})\langle 2| \\ + |2\rangle V_{21}(\hat{R})\langle 1| + |2\rangle\left(-\frac{1}{2}\nabla_R^2 + V_{22}(\hat{R})\right)\langle 2|$$

where

$$V_{11}(\hat{R}) = E_0 + \omega^2 R^2 \quad V_{22}(\hat{R}) = E_1 + \omega^2 R^2 \quad V_{12}(\hat{R}) = V_{21}(\hat{R}) = \lambda$$

- a. Determine the associated adiabatic potentials and non-adiabatic coupling. Sketch these as a function of  $R$ . Is there anything unusual here?

- b. Within the Born-Oppenheimer approximation, the total energies of the system are the eigenvalues of

$$\hat{H}_N = -\frac{1}{2}\nabla_R^2 + E_i(\mathbf{R})$$

where  $E_i(\mathbf{R})$  is one of the adiabatic potentials from the previous part. What are the Born-Oppenheimer total energies for this system? When will they be accurate?

5. (20 pts.) We're going to consider two electrons in a Harmonic potential. The position and momentum of electron 1 (2) will be denoted by  $\hat{q}_1, \hat{p}_1$  ( $\hat{q}_2, \hat{p}_2$ ).

- a. First, we will assume that the electrons do not interact. Thus the Hamiltonian is

$$\hat{H}_0 \equiv \frac{\hat{p}_1^2}{2m} + \frac{1}{2}m\omega^2 \hat{q}_1^2 + \frac{\hat{p}_2^2}{2m} + \frac{1}{2}m\omega^2 \hat{q}_2^2$$

Write down the lowest singlet and triplet energy eigenstates for the two non-interacting electrons in this potential. What are the energies of these two states?

- b. Now, assume the electrons repel each other via an interaction:

$$V \equiv e(\hat{q}_1 - \hat{q}_2)^2.$$

Treat this interaction as a perturbation and determine the first order changes in the singlet and triplet energies from part a.