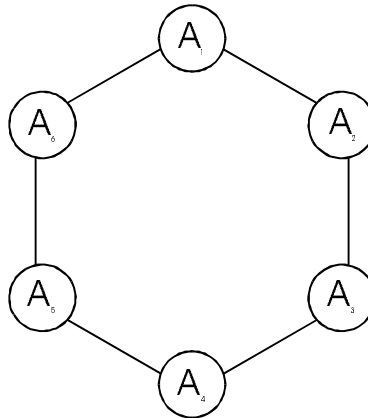


## Ph195a, study problems for 11/19/01

The following two homework problems are from Cohen-Tannoudji *et al*, Complement J<sub>IV</sub>. A molecule is composed of six identical atoms  $A_1, A_2, \dots, A_6$  which form a regular hexagon. Consider an electron which can be localized on each of the atoms. Call  $|\varphi_n\rangle$  the state in which it is localized on the  $n^{\text{th}}$  atom ( $n = 1, 2, \dots, 6$ ). The electron states will be confined to the space spanned by the  $|\varphi_n\rangle$ , assumed to be orthonormal.



1NS. Define an operator  $\mathbf{R}$  by the following relations:

$$\mathbf{R}|\varphi_1\rangle = |\varphi_2\rangle; \mathbf{R}|\varphi_2\rangle = |\varphi_3\rangle; \dots; \mathbf{R}|\varphi_6\rangle = |\varphi_1\rangle.$$

Find the eigenvalues and eigenstates of  $\mathbf{R}$ . Show that the eigenvectors of  $\mathbf{R}$  form a basis of the state space.

2NS. When the possibility of the electron passing from one site to another is neglected, its energy is described by a Hamiltonian  $\mathbf{H}_0$  whose eigenstates are the six states  $|\varphi_n\rangle$ , with the same eigenvalue  $E_0$ . We describe the possibility of the electron jumping from one atom to another by adding a perturbation  $\mathbf{W}$  to the Hamiltonian  $\mathbf{H}_0$ ;  $\mathbf{W}$  is defined by:

$$\mathbf{W}|\varphi_1\rangle = -a|\varphi_6\rangle - a|\varphi_2\rangle; \mathbf{W}|\varphi_2\rangle = -a|\varphi_1\rangle - a|\varphi_3\rangle; \dots \dots;$$

$$\mathbf{W}|\varphi_6\rangle = -a|\varphi_5\rangle - a|\varphi_1\rangle.$$

Show that  $\mathbf{R}$  commutes with the total Hamiltonian  $\mathbf{H} = \mathbf{H}_0 + \mathbf{W}$ . From this deduce the eigenstates and eigenvalues of  $\mathbf{H}$ . In these eigenstates, is the electron localized?

The following three homework problems are **modified** from Cohen-Tannoudji *et al*, Complement H<sub>XI</sub>.

Consider a system formed by an electron spin  $S$  and two nuclear spins  $I_1$  and  $I_2$  ( $S$  could be, for example, the spin of the unpaired electron of a paramagnetic diatomic molecule, and  $I_1$  and  $I_2$  the spins of the two nuclei of this molecule). Assume that  $S, I_1, I_2$  are all spin 1/2's. The state space of the three-spin system is spanned by the eight orthonormal kets  $|\varepsilon_S, \varepsilon_1, \varepsilon_2\rangle$ , common eigenvectors of  $\mathbf{S}_z, \mathbf{I}_{1z}, \mathbf{I}_{2z}$  with respective eigenvalues  $\varepsilon_S\hbar/2, \varepsilon_1\hbar/2$ , and  $\varepsilon_2\hbar/2$  (where  $\varepsilon_S = \pm 1, \varepsilon_1 = \pm 1$ , and  $\varepsilon_2 = \pm 1$ ). For example, the ket  $|+, -, +\rangle$  corresponds

to the eigenvalues  $+\hbar/2$  for  $\mathbf{S}_z$ ,  $-\hbar/2$  for  $\mathbf{I}_{1z}$ , and  $+\hbar/2$  for  $\mathbf{I}_{2z}$ .

3NS. We begin by neglecting any coupling of the three spins. We assume, however, that they are placed in a uniform magnetic field  $\vec{B}$  parallel to the  $z$  axis. Since the gyromagnetic ratios of  $I_1$  and  $I_2$  are equal, the Hamiltonian  $\mathbf{H}_0$  of the system can be written

$$\mathbf{H}_0 = \Omega \mathbf{S}_z \otimes \mathbf{1}^{nuc} + \mathbf{1}^{el} \otimes (\omega \mathbf{I}_{1z} + \omega \mathbf{I}_{2z})$$

where  $\Omega$  and  $\omega$  are real, positive constants, proportional to  $|\vec{B}|$ . Assume  $\Omega > 2\omega$ .

What are the possible energies of the three-spin system and their degrees of degeneracy? Draw the energy diagram.

4NS. We now take coupling of the spins into account by adding the Hamiltonian

$$\begin{aligned} \mathbf{W} &= a \mathbf{S} \cdot \mathbf{I}_1 - a \mathbf{S} \cdot \mathbf{I}_2 \\ &= a (\mathbf{S}_x \otimes (\mathbf{I}_{1x} - \mathbf{I}_{2x}) + \mathbf{S}_y \otimes (\mathbf{I}_{1y} - \mathbf{I}_{2y}) + \mathbf{S}_z \otimes (\mathbf{I}_{1z} - \mathbf{I}_{2z})) \end{aligned}$$

where  $a$  is a real, positive constant (the direct coupling of  $I_1$  and  $I_2$  is negligible).

What conditions must be satisfied by  $\varepsilon_S, \varepsilon_1, \varepsilon_2, \varepsilon'_S, \varepsilon'_1, \varepsilon'_2$  for  $a \mathbf{S} \cdot \mathbf{I}_1$  to have a non-zero matrix element between  $|\varepsilon_S, \varepsilon_1, \varepsilon_2\rangle$  and  $|\varepsilon'_S, \varepsilon'_1, \varepsilon'_2\rangle$ ? Same question for  $a \mathbf{S} \cdot \mathbf{I}_2$ .

5NS. Assume that

$$a\hbar^2 \ll \hbar\Omega, \hbar\omega$$

so that  $\mathbf{W}$  can be treated as a perturbation with respect to  $\mathbf{H}_0$ . To first order in  $\mathbf{W}$ , what are the eigenvalues of the total Hamiltonian  $\mathbf{H} = \mathbf{H}_0 + \mathbf{W}$ ? To zeroth order in  $\mathbf{W}$ , what are the eigenstates of  $\mathbf{H}$ ? Draw the energy diagram.