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October 2010 - Entrance Examination: Condensed Matter

Solve at least one of the following problems. Write out solutions clearly and concisely. State each approximation used. Diagrams welcome. Number page, problem, and question clearly. Do not write your name on the problem sheet, but use extra envelope.

Problem 1: A triatomic chain

Consider a simple model triatomic chain – for example three simplified "hydrogen atoms" on an equilateral triangle. Each atom is modeled as a single electron placed on an energy level e_0. From each atom, the electron can hop onto the two neighboring atoms with a matrix element $-t$, with $t > 0$. The electrons are supposed to be non interacting. The one-electron Hamiltonian is therefore

$$H_0 = e_0 \sum_i |i\rangle\langle i| - t \sum_{ij} |i\rangle\langle j|, \tag{1}$$

where $|i\rangle$ is the wavefunction on atom i, $i = 1, 2, 3$, and $j \neq i$. One can also set in full generality $e_0 = 0$, $t = 1$.

1. Diagonalize this triatomic chain Hamiltonian, find the eigenstates and their eigenfunctions, as linear combinations of the three atomic states $|1\rangle, |2\rangle, |3\rangle$.

2. Fill these eigenstates with the three electrons, keeping into account the Pauli principle, and determine all ground state properties: a) the total energy; b) the spin.

3. Now change slightly the Hamiltonian by turning the hopping energy between atoms 1 and 2 from $-t$ to $-t(1 + x)$ with x small and positive, while leaving all the rest unperturbed. Describe the perturbative change of the one electron levels, of the total energy, and of the other properties of the system.

4. Return to the unperturbed Hamiltonian and its ground state. Raise the total spin by one, and find the total energy of that excited state.

5. Show that the system is invariant for rotations of 120° around an axis perpendicular to the plane of the molecule and passing through its center. Discuss how this symmetry can be used to classify the eigenstates of the Hamiltonian using a quantum number that is analogous to a wave-vector of a finite 1D chain, and apply this classification to the ground and excited states discussed in this problem.

6. (Optional). Would it be possible to stabilize a high spin state similar to that of question (4) if one would consider the mutual repulsion of two electrons on the same atom? Elaborate on this point.

Problem 2: The Landé g factor

Let us consider an open shell atom or ion with a degenerate ground state, and indicate with $|LSJJ_z\rangle$ the degenerate wavefunctions. LSJ label the eigenvalues of $\mathbf{L}^2$, $\mathbf{S}^2$ and $\mathbf{J}^2$ where $\mathbf{L}$ is the orbital angular momentum, $\mathbf{S}$ the spin angular momentum and $\mathbf{J}$ the total angular momentum, respectively.

1. Show that the energy cannot depend on the projection of the total angular momentum along the z axis $\hbar J_z$, whose discrete allowed values are $-J \leq J_z \leq J$.

2. Show that, in addition to the magnetic moment $\boldsymbol{\mu}_S$ due to spin $\boldsymbol{\mu}_S = -g_0 \frac{e}{2m}\mathbf{S}$, the ion has a magnetic moment due to the orbital motion equal to $\boldsymbol{\mu}_L = -a\mathbf{L}$ and find the proportionality constant a in terms of the electron charge $-e$ and mass m. ($g_0 \approx 2$ is the electron gyromagnetic ratio).

3. Calculate the expectation value of $\langle LSJJ_z|(\mathbf{L} + g_0\mathbf{S})|LSJJ'_z\rangle$ and show that it is proportional to the expectation value of $\langle LSJJ_z|\mathbf{J}|LSJJ'_z\rangle$ with a proportionality factor $g(LSJ)$ independent from J_z and J'_z.

   Hint: Multiply both terms by $\langle LSJJ'_z|\mathbf{J}|LSJJ_z\rangle$ and sum over J and J'_z.

4. Which are the possible values of the energy of this ion in a magnetic field B parallel to the z axis?

   Hint: You can use first order perturbation theory to estimate the energy.

5. Calculate these values for a Ce ion with $L = 3$, $S = 1/2$, $J = 5/2$ and taking $g_0 = 2$.

Problem 3: A particle in a one-dimensional potential

A particle of mass m in one dimension is known to have a time-independent probability density distribution:

$$n(x) = c\mathrm{e}^{-2(\alpha x^2+\beta x^4)} \tag{2}$$

where c, α, and β are positive constants.

1. Write down the form of the most general wave-function compatible with the given probability distribution.

Assume now that the Hamiltonian of the system is of the form:

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \tag{3}$$

2. Show that under this assumption the wave-function previously discussed is uniquely determined and that it has to be an eigenfunction of the Hamiltonian. Explain why the above assumption on the form of the Hamiltonian is essential to draw these conclusions.

3. Discuss whether the wave-function determined above can be an excited state of the Hamiltonian or if it has to be the ground state.

4. Determine the most general from of the potential consistent with the wave-function determined above.

5. Fix the additive, arbitrary constant of the potential in such a way that$V(0) = 0$ and determine the ground-state energy corresponding to $\beta = 0$. Does the ground-state energy increase, decrease, or remain unchanged, when $\beta > 0$?

6. Suppose that $\beta \ll \alpha^2$ and determine how the first excitation energy depends on β in this limit.