SISSA ISAS

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March 2012 - 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 simple model for the Born-Oppenheimer approximation

Consider the Hamiltonian for two coupled one-dimensional oscillators:

$$\mathcal{H} = \frac{P^2}{2M} + \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \frac{1}{2}M\Omega^2 X^2 + gXx,$$

where (x, p) and (X, P) are conjugate variables that represent an electron and an ion position and momentum, respectively ($[x, p] = i$, $[R, P] = i$, $[x, X] = [p, P] = [x, P] = [X, p] = 0$).

1. Find the exact eigenvalues of $\mathcal{H}$ in terms of two quantum numbers n_1 and n_2.
2. Expand the eigenvalues in the limit of $m/M \ll 1$ and write their expression up to first order in m/M. Draw the structure of the energy levels. (Consider that $\omega^2 = k_1/m$ and $\Omega^2 = k_2/M$ where k_1 and k_2 are given constants).

Consider now the Born-Oppenheimer approximation $M \to \infty$. In this limit the electron Hamiltonian is:

$$\mathcal{H}_{el} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + gXx + \frac{1}{2}k_2 X^2.$$

3. Solve the electronic problem and find the eigenvalues $E(X)$ of $\mathcal{H}_{el}$ as a function of X.
4. Reintroduce the kinetic energy of the ions and solve the ionic problem with the electron in its ground state. (Hint: $E(X)$ acts as the potential energy for the ions)
5. Compare the Born-Oppenheimer solution with the exact results and discuss the validity of the approximation.

Problem 2: Long-range interaction between a hydrogen and an anti-hydrogen

Consider a system formed by a hydrogen (a proton and an electron) and an anti-hydrogen (an anti-proton and a positron) at a large distance R.

Assume the proton coordinates (position and momentum) are $\mathbf{R}_A$, $\mathbf{P}_A$; the anti-proton coordinates are $\mathbf{R}_B$, $\mathbf{P}_B$; the electron coordinates are $\mathbf{r}_a$, $\mathbf{p}_a$; and the positron coordinates are $\mathbf{r}_b$, $\mathbf{p}_b$. Each atom (or anti atom) is neutral and has no net dipole in its ground state, what is the interaction energy between the two atoms at large separation?

Apply the adiabatic approximation to the heavy particles and focus on the (electron-positron) system at fixed proton/anti-proton positions.

1. Write the Hamiltonian of the (electron-positron) system in terms of the above coordinates.

2. Introduce relative coordinates $\mathbf{x}_a = \mathbf{r}_a - \mathbf{R}_A$, $\mathbf{x}_b = \mathbf{r}_b - \mathbf{R}_B$, and $\mathbf{R} = \mathbf{R}_A - \mathbf{R}_B$. Rewrite the Hamiltonian of the system in the above coordinates.

3. Show that for $|\mathbf{R}| \longrightarrow \infty$ the Hamiltonian reduces to the one of two isolated atoms. Give the value of the ground state energy.

4. Expand the Hamiltonian in powers of $1/|\mathbf{R}|$ stopping at the first non vanishing term.

5. Calculate the correction to the energy computed at point 3. by applying first-order perturbation theory and show that it vanishes.

6. Evaluate formally the second-order perturbation theory contribution and show that it does not vanish.

7. What is the leading power law in the interaction between the two neutral atoms? Is the interaction always attractive, always repulsive or not defined?

Hint: the following expansion may be useful

$$\frac{1}{|\mathbf{x} + \mathbf{R}|} = \frac{1}{|\mathbf{R}|} - \frac{\mathbf{R} \cdot \mathbf{x}}{|\mathbf{R}|^3} + \frac{3(\mathbf{R} \cdot \mathbf{x})^2 - (\mathbf{x} \cdot \mathbf{x})(\mathbf{R} \cdot \mathbf{R})}{2|\mathbf{R}|^5} + \mathcal{O}(1/|\mathbf{R}|^4)$$

Problem 3: Rashba splitting

The electronic states of the surfaces of some nonmagnetic metals can be spin polarized due to spin-orbit coupling. In this problem we study some properties of these electronic states. Let us consider a two dimensional gas of independent electrons which move in a square box of edge L (L is very large) with periodic boundary conditions. The electrons have spin and interact through spin-orbit coupling with an external potential. Their behavior can be described by the Hamiltonian:

$$H = \frac{p_x^2 + p_y^2}{2m} + b\,(p_x \sigma_y - p_y \sigma_x)$$

where $\boldsymbol{\sigma}$ are the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0, & 1 \\ 1, & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0, & -i \\ i, & 0 \end{pmatrix},$$

$\mathbf{p} = -i\hbar \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right)$ is the electron momentum, m is the electron effective mass and b a positive parameter.

1. Find the band structure of this system, searching the eigenfunctions of the Hamiltonian in the form of two dimensional plane waves multiplied by two-component spinors:
$$\psi_{\mathbf{k}}(x, y) = A e^{ik_x x + ik_y y} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$$
Plot the eigenvalues $\epsilon_{\mathbf{k}}$ along the three lines $\mathbf{k} = (k, 0)$, $\mathbf{k} = (0, k)$, and $\mathbf{k} = \frac{1}{\sqrt{2}}(k, k)$ as a function of k. You can take $\hbar = 1$, $m = 1$ and b positive.

2. At the point $\mathbf{k} = (k, 0)$ find the coefficients α and β of the eigenvectors of H such that $|\alpha|^2 + |\beta|^2 = 1$. For the two eigenvectors calculate the expectation values of the spin angular momentum $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$. In which direction is the spin pointing?

3. Repeat point 2.) at the generic point $\mathbf{k} = (k\cos\theta, k\sin\theta)$. In which direction is the spin pointing?

4. Consider now the energy $E = -b^2/4$ (with the same units used at point 1.). In the plane (k_x, k_y) find the curves $\epsilon_{\mathbf{k}} = E$. In a few $\mathbf{k}$ points along these curves indicate with an arrow the direction of the expectation value of the spin on the eigenstate of H at that point. Do a similar plot for $E = b^2/4$.

Problem 4: One-dimensional scattering off a localized magnetic field

Consider spin-1/2 electrons moving in one dimension with the Hamiltonian ($\hbar = 1$):

$$\mathcal{H} = -\frac{1}{2m}\frac{d^2}{dx^2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - B\,\delta(x)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \tag{1}$$

where x is the coordinate, B the strength of a magnetic field in the x direction localized at the origin, and the matrices act on the spin up and down components of the wave function

$$\boldsymbol{\psi}(x) = \begin{pmatrix}\psi_\uparrow(x)\\ \psi_\downarrow(x)\end{pmatrix}.$$

Imagine an electron that scatters off the magnetic potential moving from $x \ll 0$, which is prepared in the state

$$\boldsymbol{\psi}_0(x \ll 0) = \mathrm{e}^{ikx}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}, \tag{2}$$

with $|\alpha|^2 + |\beta|^2 = 1$. Without loss of generality, you may take a real α.

1. Demonstrate that the scattered wave function will generally be of the form

$$\boldsymbol{\psi}(x<0) = \mathrm{e}^{ikx}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} + \mathrm{e}^{-ikx}\begin{pmatrix}\mathrm{r}_\uparrow\\ \mathrm{r}_\downarrow\end{pmatrix}, \tag{3}$$

$$\boldsymbol{\psi}(x>0) = \mathrm{e}^{ikx}\begin{pmatrix}\mathrm{t}_\uparrow\\ \mathrm{t}_\downarrow\end{pmatrix}. \tag{4}$$

   in terms of the reflection, r_σ, and transmission, t_σ, coefficients for each spin projection.

2. Write down the equations, without solving them, that r_σ and t_σ have to satisfy for the wave function Eqs. (3) and (4) to be an eigenstate of (1).

3. Solve those equations to determine α and β such that the transmitted electron has only spin down component, i.e. $\mathrm{t}_\uparrow = 0$.

4. Interpret the result by computing the expectation value of the spin operator $\mathbf{S} = \frac{\boldsymbol{\sigma}}{2}$ on the initial state.