Quantum mechanics II, Problems 8- Perturbation Theory II

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Problem 1 : Degenerate Perturbation Theory for a 3-State System

We consider the following Hamiltonian acting on a spin 1:

$$\hat{H} = -D\hat{S}_z^2 + \lambda B\hat{S}_x \tag{1}$$

This is a model that can be realistic in certain materials. The first term represents an anisotropy, and the second a magnetic field along the x direction. We propose to diagonalize this Hamiltonian by considering the term $\lambda B \hat{S}_x$ as a perturbation. Subsequently, we assume that B and D are non-zero. Reminder from "quantum physics 1" course: For a spins s, we have $\hat{S}_z | s, m \rangle = \hbar m | s, m \rangle$ with $-s \leq m \leq s$. And the raising/lowering operators $\hat{S}_{\pm} = \hat{S}_x \pm i \hat{S}_y$ acting on these eigenvectors gives $\hat{S}_{\pm} | s, m \rangle = \sqrt{s(s+1) - m(m\pm 1)} | s, m \pm 1 \rangle$.

- 1. Under what condition does the Hamiltonian commute with \hat{S}_z ? In this case, give the eigenvalues and eigenvectors of \hat{H} .
- 2. Subsequently, we consider $\lambda \neq 0$. Write down the matrix of the Hamiltonian in the basis of eigenstates of \hat{S}_z . Using second order perturbation theory, compute the energy correction for the state $|m=0\rangle$. Calculate the correction to the associated eigenvector, to first order in perturbation theory.
- 3. To calculate the effect of the perturbation on the other two states, it is necessary to use degenerate perturbation theory. What is the matrix of the operator \hat{S}_x in the degenerate subspace? Deduce that the first-order correction is zero.

<u>Problem 2</u>: Hydrogen atom in an external magnetic field

The Hamiltonian of a hydrogen atom under a weak uniform magnetic field directed along the z axis can be expressed as

$$H = \frac{(\mathbf{p} + e\mathbf{A})^2}{2m} - \frac{e^2}{|\mathbf{r}|} - \boldsymbol{\mu} \cdot \mathbf{B} . \tag{2}$$

Here $\boldsymbol{\mu} = 2\mu_e \mathbf{s}$, with μ_e the electron magnetic moment and \mathbf{s} the electron spin. Using the radial gauge $\mathbf{A} = \frac{1}{2}(-By, Bx, 0) = \frac{1}{2}\mathbf{B} \times \mathbf{r}$, and neglecting, for small B, terms of order B^2 , the Hamiltonian can then be rewritten as

$$H = \frac{\mathbf{p}^{2}}{2m} - \frac{e^{2}}{|\mathbf{r}|} + \frac{e}{2m}(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) - 2\mu_{e}\mathbf{s} \cdot \mathbf{B}$$

$$= H_{0} + \frac{e}{4m}(\mathbf{p} \cdot (\mathbf{B} \times \mathbf{r}) + (\mathbf{B} \times \mathbf{r}) \cdot \mathbf{p}) - 2\mu_{e}\mathbf{s} \cdot \mathbf{B}$$

$$= H_{0} + \frac{e\hbar}{2m}\mathbf{B} \cdot \ell - 2\mu_{e}\mathbf{s} \cdot \mathbf{B}$$
(3)

where $H_0 = H|_{B=0}$ Calculate the splitting of the hydrogen energy levels to first order in **B**.

Hint. By rotational invariance, the spectrum cannot depend on the direction of the magnetic field. This invariance can be used to simplify the calculations.

Problem 3: Perturbed two-dimensional harmonic oscillator

Consider a two-dimensional harmonic oscillator governed by the Hamiltonian

$$H = H_0 + gH_1$$
, $H_0 = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega^2(x^2 + y^2)$, $H_1 = x^2y^2$. (4)

The model, for example, can describe in an approximate way an optical phonon in a two dimensional lattice with square anisotropy.

- 1. Consider the unperturbed Hamiltonian H_0 , which describes a two-dimensional harmonic oscillator. Describe the spectrum of H_0 , expressing the eigenstates and the corresponding energies.
- 2. Study how the ground state, the first excited level, and the second excited level of the unpertubed Hamiltonian are modified by H_1 , using perturbation theory to first order in g.

 Hint. It is convenient to express x and y in terms of the ladder operators for the harmonic oscillator.