

Exercise sheet XI

due 27.5.2008.

Problem 1 [*Anharmonic oscillator*]: Consider the Hamilton operator of the anharmonic oscillator in one dimension,

$$H = H_0 + H_a, \quad H_0 = -\frac{\hbar^2}{2m}\Delta + \frac{1}{2}m\omega^2x^2, \quad H_a = \lambda \left(\frac{x}{x_0}\right)^4, \quad (1)$$

where $x_0 = \sqrt{\frac{\hbar}{m\omega}}$. The aim of this question is to determine the energy spectrum of the anharmonic oscillator in 2nd-order perturbation theory.

(i) Express H in terms of the creation and annihilation operators of the harmonic oscillator.

(ii) Determine the matrix elements of H_a in the eigenbasis of the harmonic oscillator, denoted by $|n\rangle$ with $n = 0, 1, 2, \dots$

(iii) Calculate the eigenvalues of H to 2nd-order perturbation theory.

(iv) The relative corrections diverge for large energies (*i.e.* for large n). For these eigenstates, perturbation theory is therefore not particularly useful. Explain why this had to be expected.

Problem 2 [*Spin-orbit coupling and Zeemann effect*]: Consider an electron in a hydrogen atom in the presence of a constant magnetic field \vec{B} , which we take to be parallel to the z -axis. Without the magnetic field and ignoring the spin orbit coupling, the eigenfunctions are labelled by (n, l, m, m_s) , where m_s denotes the spin quantum number $m_s = \pm\frac{1}{2}$. The additional effects lead to $H = H_0 + \Delta H$ with

$$\Delta H = \kappa \vec{L} \cdot \vec{S} + \mu_B B_z (L_z + 2S_z), \quad (2)$$

where $\kappa = \frac{1}{2m^2c^2} \langle \frac{1}{r} \frac{dV}{dr} \rangle_{n,l}$ and $\mu_B = \frac{e\hbar}{2mc}$ is the Bohr magneton.

(i) If the second term dominates (Paschen-Back effect), determine the first order perturbation of the energy spectrum, treating only the spin-orbit coupling as a perturbation. How big does B_z have to be in order to justify this approximation?

(ii) Next, determine the energy spectrum to first order perturbation theory treating both terms (*i.e.* ΔH) as a perturbation. [*Hint*: To this end you need to diagonalise the $2(2l+1) \times 2(2l+1)$ matrix, where $m = -l, \dots, l$ and $m_s = \pm\frac{1}{2}$. Since $[L_z + S_z, \Delta H] = 0$, this matrix is already blockdiagonal.]

(iii) For $B_z = 0$ reproduce the result for the spin orbit coupling that was derived in the lectures. Show that the first order correction in B_z of this result is given by

$$\Delta E_{nljm_j} = g_{lj} \mu_B B_z m_j, \quad m_j = -j, \dots, j, \quad (3)$$

where j and m_j refer to the diagonal representation of the rotation group corresponding to $\vec{J} = \vec{L} + \vec{S}$. Here,

$$g_{l,l+1/2} = \frac{2+2l}{1+2l}, \quad g_{l,l-1/2} = \frac{2l}{1+2l}.$$

Problem 3 [*Degenerated perturbation theory*]: A quantum system with a 3-dimensional space of states has the Hamiltonian H , which in matrix representation is given as

$$H = \begin{pmatrix} \mathcal{E}_1 & 0 & a \\ 0 & \mathcal{E}_1 & b \\ a^* & b^* & \mathcal{E}_2 \end{pmatrix}, \quad \mathcal{E}_2 - \mathcal{E}_1 > 0 .$$

We want to think of $\mathcal{E}_{1,2}$ as the eigenvalues of the unperturbed system, and of a, b , as small ($a, b \ll \mathcal{E}_2 - \mathcal{E}_1$) matrix elements describing the perturbation. Calculate the perturbed eigenvalues via

- (i) second-order nondegenerate perturbation theory — where does it fail?
- (ii) second-order degenerate perturbation theory.

Finally, calculate the exact energies and compare your results.