Advanced Quantum Mechanics WS 2024/25, Problem set 4

Final version

We use $\hbar = 1$ in these exercises

4.1 Two electrons with spin in an harmonic oscillator

Consider two electrons with spin $\frac{1}{2}$ in an (slightly modified) harmonic oscillator. The system is described by the Hamiltonian

$$H_0 = H_1 + H_2 \qquad H_i = \omega \left(a_i^\dagger a_i + 1\right)$$

where $a_i^\dagger$, a_i are the creation and annihilation operators for particle i (i=1,2).

(a) By initially neglecting the interaction between the electrons, write down the two-particle ground state $|G\rangle$ and the (degenerate) first excited state(s) $|E_i\rangle$ together with their (eigen-)energies and degeneracies.

Express the states as tensor products of an orbital (= spatial) and a spin part, similarly to the treatment of Helium in class: i.e. the orbital part as a suitably (anti)symmetrized combination of tensor products of harmonic oscillator levels $|n_1\rangle |n_2\rangle$ ($n_i = 0, 1, \cdots, \infty$) and the spin part as a total spin (= total internal angular momentum) eigenstate $|S, m\rangle$.

(b) We now introduce the interaction between the two electrons as

$$\hat{V} = \alpha\ \hat{x}_1 \hat{x}_2 \equiv \hat{V}_{Orb} \otimes \mathbb{I}_S\ ,$$

where $\hat{x}_i$ is the position operator of particle i.

(c) Evaluate all matrix elements of $\hat{V}$ between the states $|E_i\rangle$

(d) Evaluate the first-order correction to the energy of the first excited states. You will have to use degenerate perturbation theory. What degeneracy is left?

4.2 cont: Spin interactions

(a) Write down the next set [1] of degenerate excited states $|F_i\rangle$ of the noninteracting harmonic oscillator of the previous exercise, along with their eigenenergy and degeneracy.

(b) The interaction is now slightly modified to

$$\hat{V} = \alpha\ \hat{x}_1 \hat{x}_2\ \mathbf{S}_1 \cdot \mathbf{S}_2 \equiv \hat{V}_{Orb} \otimes \hat{V}_S\ ,$$

where $\mathbf{S}_i$ are the spin operators of the two particles.

Determine which matrix elements of $\hat{V}$ between the states $|F_i\rangle$ are expected to be nonzero and which ones are equal to each other. Use rotation symmetries (Wigner Eckart theorem)

4.3 cont: degenerate perturbation theory

Evaluate the correction to the energy of the $|F_i\rangle$ states to first order in α. What degeneracies are left?

Hints for the exercises above: (i) To determine the noninteracting states, first write down a level diagram and think about the possible combinations compatible with Pauli principle. Don't forget the spin.

(ii) Express the position operators x_i in terms of the a_i and $a_i^\dagger$ operators of the harmonic oscillator.

(iii) Notice that $\mathbf{S}_1 \cdot \mathbf{S}_2$ is diagonal in the total spin eigenstates.

(iv) Remember: in degenerate perturbation theory you need in principle to determine

[1] The ones which have eigenenergies just above the ones of the $|E_i\rangle$.

all matrix elements of $\hat{V}$ within the subspace of the degenerate eigenstates and then diagonalize this matrix. **However:** notice that most matrix elements are zero. Thus, first of all identify between which states $\hat{V}$ is zero, especially looking at the spin part of those matrix elements. You should be able to determine the matrix elements of $\hat{V}_S$ essentially without any calculation.

(v) For an efficient evaluation of the matrix elements of $\hat{V}_{Orb}$ I suggest the following: (a) apply $\hat{V}_{Orb}$ to each orbital state and (b) neglect all terms that fall outside of the degenerate subspace. (c) Try to write the resulting state in terms of another state in the degenerate subspace.