List of exercises #6 - 7600037

1. In a system of identical particles,
   (a) Show that $\langle \Psi | O | \Psi \rangle = \left\langle \Psi \left| P_{ij}^{\dagger} O P_{ij} \right| \Psi \right\rangle$, where $|\Psi\rangle$ is a physical state, O is an observable, and P_{ij} is the permutation operator of particles i and j.
   (b) A consequence of the previous item is that $[O, P_{ij}] = 0$. What is the meaning of this relation to physical observables? Does the operator S_i^z commute with the permutation operator? Does $\sum_i S_i^z$ commute with the permutation operator? Interpret your answers.
   (c) Let $|S\rangle$ and $|A\rangle$ be totally symmetric and antisymmetric states, respectvely. Show that $\langle S | O | A \rangle = 0$.
   (d) Show that, if $P_{ij} |\Psi_0\rangle = \alpha |\Psi_0\rangle$ (with $\alpha = \pm 1$), then $P_{ij} |\Psi_t\rangle = \alpha |\Psi_t\rangle$, where $|\Psi_t\rangle = U(t, 0) |\Psi_0\rangle$ and $U(t, 0)$ is the time-evolution operator. Interpret this result.

2. Consider a one-particle quantum mechanical system with a Hilbert space spanned by three orthonormal states $|n\rangle$, with $n = 1, 2, 3$. Three non-interacting particles occupy these states. Determine how many distinct physical states there are if these particles are (neglect their spin):
   (a) three identical fermions,
   (b) three identical bosons,
   (c) two identical fermions and one boson,
   (d) two identical bosons and one fermion,
   (e) three distinct fermions, and
   (f) three distinct bosons.

3. Same as the previous problem, but for 3 identical spin-1/2 particles. In each case, classify the corresponding orbital states with respect to all possible permutations. Is there a orbital state which has mixed symmetry? That is, it is neither totally symmetric or antisymmetric with respect to permutations (when the spin degrees of freedom are ignored)?

4. Three identical spin-0 particles are located at the corners of an equilateral triangle. The system is free to rotate about an axis that goes through the center of the triangle and is perpendicular to it (say, the z-axis). Due to the symmetry of the many-particle wavefunction, what are the restrictions on the z-projection of the total orbital angular momentum J^z? (Recall that the total angular momentum is the generator of the rotations.)

5. The purpose of this problem is to understand the exchange interaction: the mechanism that gives stability to the Hydrogen molecule and the covalent bond, among other things such as magnetism.
   (a) Write the complete Hamiltonian H of the Hydrogen molecule.
   (b) In the limit the two protons are faraway from each other, $R \gg a_0$, with a_0 being the Bohr radius, write $H = H_0 + W$ with H_0 and W being the nonperturbed Hamiltonian and its perturbation, respectively. Justify your choice of H_0 and W.
   (c) Now, use the limit in which the protons are much heavier than the electrons. What is the physical meaning of this limit? Moreover, consider the protons being classical particles (thus, R becomes a parameter in the problem) and treat the electrons as indistinguishable spin-1/2 quantum particles. Write the simplified H_0 and W.
   (d) Write down the ground-state wavefunctions of H_0 (do not forget the spin and the normalization). What is the degeneracy of the ground state? Discuss the permutation properties of the ground-state wavefunctions.
   (e) In first order of perturbation theory, compute the correction to the ground-state energy ΔE due to W, and analyze how the degeneracy is lifted. (Do not compute the integrals. Just analyze how they can lift the degeneracy.)
   (f) Which is the new ground state? Discuss its symmetry properties and the role of the parameter R. (As the integrals in the previous item (e) were not computed, you cannot decide for which one. Thus, discuss all the possible outcomes. Can give a physical insight to decide if the integral is positive or negative?)
      i. (Optional) Compute the integrals. (All of them, but one, can be computed analytically. Perform the remaining one numerically.)

(g) What is the condition that ΔE must satisfy in order to guarantee the stability of the Hydrogen molecule?

(h) Notice that the degeneracy of the ground state is lifted in a way that the new spectrum can be represented by the effective Hamiltonian $H_{\text{eff}} = \text{const} + J\mathbf{S}_1 \cdot \mathbf{S}_2$, where $\mathbf{S}_i$ is the spin operator of the i-th electron. Give the expression for the exchange coupling J.

(i) Notice that $J\mathbf{S}_1 \cdot \mathbf{S}_2$ is a magnetic type interaction (two dipoles interacting). However, the Hamiltonian is purely electric. Discuss which physical principle (or principles) is (are) involved in order to give an effective magnetic interaction from "purely" electric interactions.

6. Let $P_{1,2}^{(\text{spin})}$ be the spin-permutator operator that exchanges the spin states of two particles, i.e., $P_{1,2}^{(\text{spin})} |s_\alpha, s_\beta\rangle = |s_\beta, s_\alpha\rangle$. Show that, for spin-1/2 particles, $P_{1,2}^{(\text{spin})} = \frac{1}{2} + \frac{2}{\hbar^2}\mathbf{S}_1 \cdot \mathbf{S}_2$.

7. Consider a two-level system the single-particle Hamiltonian of which is

$$H = \epsilon_{\text{A}} |A\rangle \langle A| + \epsilon_{\text{B}} |B\rangle \langle B| + V |A\rangle \langle B| + V^* |B\rangle \langle A| ,$$

where $|A\rangle$ and $|B\rangle$ are the associated states of these two levels, $\epsilon_{A,B}$ are the corresponding energies, and V is the corresponding hybridization.

(a) Write down the matrix whose eigenvalues are the eigenenergies of this single-particle Hamiltonian. What are the corresponding eigenenergies?

(b) What is the Hamiltonian (and the corresponding matrix) when there are two non-interacting spin-1 bosons? What are the corresponding eigenenergies?

(c) Show that the eigenenergies are those obtained from a simple sum of the single-particle eigenenergies. Why is this the case?

(d) Consider now the case in which there is an additional energy, say, equal to U, when both particles are in the same orbital state $|A\rangle$. What are the corresponding eigenenergies?

8. Consider a system of three equivalent orbital states $\{|i\rangle\}$, $i = 1, 2, 3$. The single-particle Hamiltonian is

$$H = -t \sum_{i \neq j} |i\rangle \langle j| = -t \left(|1\rangle \langle 2| + |1\rangle \langle 3| + |2\rangle \langle 3| + \text{h.c.} \right) .$$

(a) Write down the matrix whose eigenvalues are the eigenenergies of this single-particle Hamiltonian.

(b) Consider now a system of two non-interacting spinless fermions in occupying these three orbitals. What are the physical states?

(c) Write down the matrix whose eigenvalues are the eigenenergies of this two-particle Hamiltonian. What is the Fermi energy? Show that the eigenenergies are those obtained from a simple sum of the single-particle eigenenergies. Why is this the case?

(d) Consider now the case of three spinless fermions and redo itens (b) and (c).