IF/UFRJ
Graduate Quantum Mechanics I
2023/2 – Raimundo

Problem Set #13

1/11/2023 - due by 13/11/2023 at 12:00 noon

1. Consider the Hamiltonian for the electron in the Hydrogen atom,

$$\mathcal{H} = \frac{p^2}{2m} - \frac{e^2}{r} + \lambda_B \mathcal{H}_B + \lambda_{SO} \mathcal{H}_{SO}, \tag{1}$$

where

$$\mathcal{H}_B = -\frac{e}{2mc}(\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{B} \tag{2}$$

represents the interaction with an external magnetic field $\mathbf{B}$ ($\mathbf{L}$ and $\mathbf{S}$ are orbital and spin angular momentum operators), and

$$\mathcal{H}_{SO} = f(r)\, \mathbf{L} \cdot \mathbf{S} \tag{3}$$

is the spin-orbit coupling, with $f(r)$ being a function solely of $r = |\mathbf{r}|$; the constants λ_B and λ_{SO} may take on the values 1 or 0, respectively representing the presence or absence of the corresponding terms. In what follows, we ignore any accidental degeneracies. Determine which values λ_B and λ_{SO} must assume so that each of the following symmetries is respected:

(a) rotation solely of the orbital variables around any axis;

(b) global rotation (*i.e., of the orbital and spin variables simultaneously*) around any axis;

(c) global rotation around an axis parallel to $\mathbf{B}$;

(d) spatial reflection;

(e) time reversal.

In some of the situations described above, the eigenstates of $\mathcal{H}$ are characterised by $|n\ell m_\ell s m_s\rangle$, respectively representing the quantum numbers associated with $\mathcal{H}_0$ (i.e. the Hamiltonian without the H_B and H_{SO} corrections), L^2, L_z, S^2, and S^z. Now we want to determine selection rules for matrix elements of the type $\langle n\ell m_\ell s m_s|\mathbf{r}|n'\ell' m'_\ell s m'_s\rangle$.

(f) Obtain the restrictions on $\Delta m_s = m_s - m'_s$ so that the matrix element is non-zero;

(g) Explore the fact that $\mathbf{r}$ is a tensor operator to impose restrictions on the possible values of $\Delta\ell = \ell - \ell'$ and of $\Delta m_\ell = m_\ell - m'_\ell$. Suppose spatial reflection is yet another symmetry of the problem, and impose further restrictions on the possible values of $\Delta\ell$.

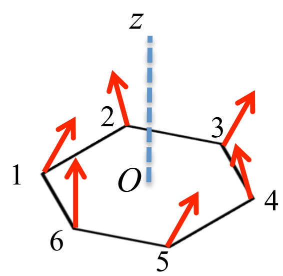

Figure 1: Problem 2 – Interacting spins-1/2 fixed attached to the vertices of a hexagon.

2. Six spin-1/2 particles are fixed in position on the vertices of a hexagon; see Fig. 1. The interactions amongst the spins and with an external magnetic field, $\mathbf{B} = B\hat{\mathbf{z}}$, are described by the Hamiltonian

$$\mathcal{H} = -\frac{J}{2}\sum_{i=1}^{6}\left[(1-\lambda)\left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right) + (1+\lambda) S_i^z S_{i+1}^z\right] - B\sum_{i=1}^{6} S_i^z,$$

where the $\mathbf{S}_i$, $i = 1, 6$ are spin operators, and it is uderstood that $\mathbf{S}_7 \equiv \mathbf{S}_1$; J is the exchange constant [units of (energy/$\hbar^2$)], λ is a dimensionless constant measuring the degree of spin anisotropy, and B has units of (energy/$\hbar$). [*Hint: try to answer as many items below as possible without evaluating commutators.*]

(a) Is $S^z \equiv \sum_{i=1}^{6} S_i^z$ a constant of motion?

(b) What values of λ and B leave $\mathcal{H}$ invariant when a rotation around Oz by an arbitrary angle is performed on all spins?

(c) What values of λ and B leave $\mathcal{H}$ invariant when a rotation around Ox by an arbitrary angle is performed on all spins?

(d) What values of λ and B leave $\mathcal{H}$ invariant under time reversal?

(e) What symmetry operations on the hexagon leave $\mathcal{H}$ invariant?

3. Let $\mathbf{A}$ be an operator whose components satisfy the commutation relations $[L_i, A_j] = i\varepsilon_{ijk}A_k$, where $\mathbf{L}$ is the orbital momentum operator. Consider the matrix elements of $\mathbf{A}$ between states $|n\ell m_\ell s m_s\rangle$ and $|n'\ell' m'_\ell s m'_s\rangle$, where n and n' are quantum numbers associated with the energy, (ℓ, m_ℓ) and (ℓ', m'_ℓ) are quantum numbers associated with the orbital angular momentum, and s, m_s and m'_s are quantum numbers associated with the spin angular momentum. Obtain the selection rules for these matrix elements of $\mathbf{A}$ in the following cases:

(a) $\mathbf{A}$ is a polar operator (*i.e.*, $\mathbf{A} \longrightarrow -\mathbf{A}$, under a spatial reflection).

(b) $\mathbf{A}$ is an axial operator (*i.e.*, $\mathbf{A} \longrightarrow \mathbf{A}$, under a spatial reflection).

4. Two particles of mass m interact through a one-dimensional harmonic potential,

$$V = \frac{1}{2}k(x_1 - x_2)^2, \quad k > 0. \tag{1}$$

Knowing that the total linear momentum of the system is zero, determine the possible energies of the system in the following cases:

(a) distinguishable particles;

(b) spinless indistinguishable particles;

(c) indistinguishable spin-1/2 particles in a singlet state;

(d) indistinguishable spin-1/2 particles in a triplet state.

5. Consider a system of two interacting fermions, and the Hamiltonian

$$\begin{aligned}\mathcal{H} = {} & A(\mathbf{S}_1 \cdot \mathbf{r})(\mathbf{S}_2 \cdot \mathbf{r}) + B(\mathbf{S}_1 \cdot \mathbf{p})(\mathbf{S}_2 \cdot \mathbf{p}) + C(S_1^z + S_2^z)(\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}) \\ & + D(\mathbf{S}_1 \cdot \mathbf{L})(\mathbf{S}_2 \cdot \mathbf{L}) \\ & + E[(\mathbf{S}_1 \cdot \mathbf{r})(\mathbf{S}_2 \cdot \mathbf{p}) + (\mathbf{S}_2 \cdot \mathbf{p})(\mathbf{S}_1 \cdot \mathbf{r}) + (\mathbf{S}_1 \cdot \mathbf{p})(\mathbf{S}_2 \cdot \mathbf{r}) + (\mathbf{S}_2 \cdot \mathbf{r})(\mathbf{S}_1 \cdot \mathbf{p})] \\ & + F(\mathbf{S}_1 \times \mathbf{S}_2) \cdot \mathbf{L} + G(\mathbf{S}_1 - \mathbf{S}_2) \cdot \mathbf{L},\end{aligned}$$

where $\mathbf{S}_i$, $i = 1, 2$, is the spin operator of particle i, and $\mathbf{r}$, $\mathbf{p}$ and $\mathbf{L}$ are the relative position, linear momentum, and angular momentum, respectively. Determine which coefficients in the above Hamiltonian must vanish so that

(a) the system is invariant under any rotations;

(b) the system is invariant under spatial reflection (through the origin);

(c) the system is invariant under time reversal;

(d) the system is invariant under the previous three transformations, and, in addition, $\mathcal{H}$ does not connect singlet and triplet states.

6. Three spins-1/2 are fixed in position on the vertices of an equilateral triangle. Each spin interacts with its nearest neighbours only (exchange coupling J), and with an external transverse field (Γ), such that the Hamiltonian can be written as

$$\mathcal{H} = -\Gamma(\sigma_1^x + \sigma_2^x + \sigma_3^x) - J(\sigma_1^z\sigma_2^z + \sigma_2^z\sigma_3^z + \sigma_3^z\sigma_1^z), \qquad (1)$$

where the σ's are Pauli matrices, so that both Γ and J have units of energy.

(a) Define an operator $R \equiv \sigma_1^x\sigma_2^x\sigma_3^x$. Show that $R^\dagger\sigma_i^z R = -\sigma_i^z$, $i = 1, 2, 3$. Compare with the effect of the operator generating a rotation of π around the direction of the transverse field. What are the eigenvalues, r, of R?

(b) Let T be a discrete translation operator, i.e. one that takes each $\boldsymbol{\sigma}_i \to \boldsymbol{\sigma}_{i+1}$, with $\boldsymbol{\sigma}_4 \equiv \boldsymbol{\sigma}_1$. What are the eigenvalues, t, of T? Verify that the sum of these eigenvalues vanishes identically.

(c) Show that T and R commute with each other.

(d) Show that $\mathcal{H}$ is invariant under R and T.

(e) Use the eigenvectors of R to set up orthonormal basis states which are simultaneous eigenstates of R and T, and express the Hamiltonian matrix in this basis.

(f) Obtain *all* energy eigenvalues, E, and sketch $E/J \times \Gamma/J$. Discuss physically the limiting cases $\Gamma \ll J$ and $G \gg J$ for the ground state.