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

Problem Set #7

18/9/2023 - due by 25/9/2023 at 12:00 noon

1. A spin-1/2 particle has a magnetic moment $\boldsymbol{\mu} = \gamma \mathbf{S}$, where $\mathbf{S}$ is the spin operator and γ is the gyromagnetic ratio. The spin space is described by the kets $|+\rangle$ and $|-\rangle$, eigenstates of S^z with eigenvalues $\pm\hbar/2$. At the instant $t = 0$ the system is in the state
$$|\psi(t = 0)\rangle = |+\rangle. \tag{1}$$

   (a) If the observable S^x is measured at $t = 0$, which results can be obtained, and with what probabilities?

   (b) Instead of performing the measurement in the previous item, we let the system evolve under the influence of a magnetic field pointing along Oy, with magnitude B_0. Determine the state of the system (in the basis $\{|\pm\rangle\}$) at an instant t.

   (c) At this instant t, we measure the observables S^x, S^y and S^z. What values can we find, and with what probabilities? What relation between B_0 and t must be satisfied so that the result of one of the measurements is certain? Can you provide a physical interpretation for this condition?

2. Consider a spin-1/2 particle with a magnetic moment $\boldsymbol{\mu} = \gamma \mathbf{S}$, where $\mathbf{S}$ is the spin operator and γ is the gyromagnetic ratio, in the presence of a magnetic field $\mathbf{B}_0$, with components $B_x = -\omega_x/\gamma$, $B_y = -\omega_y/\gamma$, and $B_z = -\omega_z/\gamma$. Let us define $\omega_0 = -\gamma|\mathbf{B}_0|$.

   (a) Show that the time evolution operator for this spin is $U(t, 0) = \mathrm{e}^{-i\Omega t}$, with
$$\Omega = \frac{1}{\hbar}\left[\omega_x S^x + \omega_y S^y + \omega_z S^z\right] = \frac{1}{2}\left[\omega_x \sigma^x + \omega_y \sigma^y + \omega_z \sigma^z\right]. \tag{1}$$

Calculate the matrix representing Ω in the basis $\{|\pm\rangle\}$ of eigenstates of S^z. Show that

$$\Omega^2 = \frac{1}{4}\left[\omega_x^2 + \omega_y^2 + \omega_z^2\right] \mathbb{1} = \left(\frac{\omega_0}{2}\right)^2 \mathbb{1}. \tag{2}$$

(b) Express the evolution operator in the form

$$U(t,0) = \cos\left(\frac{\omega_0 t}{2}\right) - \frac{2i}{\omega_0}\,\Omega \sin\left(\frac{\omega_0 t}{2}\right). \tag{3}$$

(c) Consider a spin which, at instant $t = 0$, is in the state $|\psi(0)\rangle = |+\rangle$. Show that the probability $\mathcal{P}_{++}(t)$ of finding it in the state $|+\rangle$ at time t is

$$\mathcal{P}_{++}(t) = |\langle +|U(t,0)|+\rangle|^2, \tag{4}$$

and obtain the relation

$$\mathcal{P}_{++}(t) = 1 - \frac{\omega_x^2 + \omega_y^2}{\omega_0^2} \sin^2\left(\frac{\omega_0 t}{2}\right). \tag{5}$$

Provide a geometrical interpretation.

3. Consider a system composed by two spins-1/2, $\mathbf{S}_1$ and $\mathbf{S}_2$, and the basis composed by the four kets $|\pm,\ \pm\rangle$. At the instant $t = 0$ the system is in the state

$$|\psi(0)\rangle = \frac{1}{2}|++\rangle + \frac{1}{2}|+-\rangle + \frac{1}{\sqrt{2}}|--\rangle. \tag{1}$$

(a) At time $t = 0$ one measures S_1^z; what is the probability of finding $-\hbar/2$? What is the state of the system after this measurement? If we then measure S_1^x, what results can be found and with what probabilities? Answer the same questions for the case in which the measurement of S_1^z led to $+\hbar/2$.

(b) Now suppose that when the system is in the state $|\psi(0)\rangle$ described above, S_1^z and S_2^z are simultaneously measured. What is the probability of finding identical results? And opposite results?

(c) Suppose that instead of performing the previous measurements, we let the system evolve under the influence of the Hamiltonian

$$\mathcal{H} = \omega_1 S_1^z + \omega_2 S_2^z. \tag{2}$$

What is the state of the system at time t? Evaluate the expectation values $\langle \mathbf{S}_1\rangle$ and $\langle \mathbf{S}_2\rangle$. Provide a physical interpretation.

(d) Show that the magnitude of the vectors $\langle \mathbf{S}_1 \rangle$ and $\langle \mathbf{S}_2 \rangle$ are smaller than $\hbar/2$. What must be the form of $|\psi(0)\rangle$ so that each of these magnitudes is equal to $\hbar/2$?

4. A molecule consists of six atoms fixed in position, forming a regular hexagon. An electron can be localised in each atom, and let $|\phi_n\rangle$ be the state in which the localisation occurs in atom n, $n = 1, 2, \ldots 6$. The electronic states are restricted to the space spanned by the kets $|\phi_n\rangle$, assumed orthonormalised.

   (a) Define an operator R through the following relations

   $$R|\phi_1\rangle = |\phi_2\rangle,\ R|\phi_2\rangle = |\phi_3\rangle, \ldots,\ R|\phi_6\rangle = |\phi_1\rangle. \tag{1}$$

   Determine the eigenvalues and eigenvectors of R. Show that these eigevectors form a basis in the state space.

   (b) When we neglect the hopping of the electron between the atoms, the system is described by a Hamiltonian $\mathcal{H}_0$, whose eigenvectors are the $|\phi_n\rangle$, all with the same energy E_0. The electron hopping can be described by a perturbation W, given by

   $$W|\phi_n\rangle = -\lambda\left(|\phi_{n-1}\rangle + |\phi_{n+1}\rangle\right);\ |\phi_7\rangle \equiv |\phi_1\rangle,\ \text{and}\ |\phi_0\rangle \equiv |\phi_6\rangle. \tag{2}$$

   Show that R commutes with the total Hamiltonian, $\mathcal{H} = \mathcal{H}_0 + W$. Use this fact to determine the eigenvectors and eigenvalues of $\mathcal{H}$; in these eigenstates, is the electron localised? Apply these ideas to the benzene molecule.