Complement J_{IV}

EXERCISES

1. Consider a spin 1/2 particle of magnetic moment $\mathbf{M} = \gamma\mathbf{S}$. The spin state space is spanned by the basis of the $|+\rangle$ and $|-\rangle$ vectors, eigenvectors of S_z with eigenvalues $+\hbar/2$ and $-\hbar/2$. At time $t = 0$, the state of the system is:

$$|\psi(t = 0)\rangle = |+\rangle$$

a. If the observable S_x is measured at time $t = 0$, what results can be found, and with what probabilities?

b. Instead of performing the preceding measurement, we let the system evolve under the influence of a magnetic field parallel to Oy, of modulus B_0. Calculate, in the $\{|+\rangle, |-\rangle\}$ basis, the state of the system at time t.

c. At this time t, we measure the observables S_x, S_y, S_z. What values can we find, and with what probabilities? What relation must exist between B_0 and t for the result of one of the measurements to be certain? Give a physical interpretation of this condition.

2. Consider a spin 1/2 particle, as in the previous exercise (using the same notation).

a. At time $t = 0$, we measure S_y and find $+\hbar/2$. What is the state vector $|\psi(0)\rangle$ immediately after the measurement?

b. Immediately after this measurement, we apply a uniform time-dependent field parallel to Oz. The Hamiltonian operator of the spin $H(t)$ is then written:

$$H(t) = \omega_0(t)\, S_z$$

Assume that $\omega_0(t)$ is zero for $t < 0$ and $t > T$ and increases linearly from 0 to ω_0 when $0 \leqslant t \leqslant T$ (T is a given parameter whose dimensions are those of time). Show that at time t the state vector can be written:

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left[e^{i\theta(t)}|+\rangle + i\, e^{-i\theta(t)}|-\rangle\right]$$

where $\theta(t)$ is a real function of t (to be calculated by the student).

c. At a time $t = \tau > T$, we measure S_y. What results can we find, and with what probabilities? Determine the relation which must exist between ω_0 and T in order for us to be sure of the result. Give the physical interpretation.

3. Consider a spin 1/2 particle placed in a magnetic field $\mathbf{B}_0$ with components:

$$\begin{cases} B_x = \dfrac{1}{\sqrt{2}} B_0 \\ B_y = 0 \\ B_z = \dfrac{1}{\sqrt{2}} B_0 \end{cases}$$

The notation is the same as that of exercise (1).

a. Calculate the matrix representing, in the $\{ | + \rangle, | - \rangle \}$ basis, the operator H, the Hamiltonian of the system.

b. Calculate the eigenvalues and the eigenvectors of H.

c. The system at time $t = 0$ is in the state $| - \rangle$. What values can be found if the energy is measured, and with what probabilities?

d. Calculate the state vector $| \psi(t) \rangle$ at time t. At this instant, S_x is measured; what is the mean value of the results that can be obtained? Give a geometrical interpretation.

4. Consider the experimental device described in §B-2-b of chapter IV (*cf.* fig. 8): a beam of atoms of spin 1/2 passes through one apparatus, which serves as a "polarizer" in a direction which makes an angle θ with Oz in the xOz plane, and then through another apparatus, the "analyzer", which measures the S_z component of the spin. We assume in this exercise that between the polarizer and the analyzer, over a length L of the atomic beam, a magnetic field $\mathbf{B}_0$ is applied which is uniform and parallel to Ox. We call v the speed of the atoms and $T = L/v$ the time during which they are submitted to the field $\mathbf{B}_0$. We set $\omega_0 = -\gamma B_0$.

a. What is the state vector $| \psi_1 \rangle$ of a spin at the moment it enters the analyzer?

b. Show that when the measurement is performed in the analyzer, there is a probability equal to $\frac{1}{2}(1 + \cos\theta \cos\omega_0 T)$ of finding $+\hbar/2$ and $\frac{1}{2}(1 - \cos\theta\cos\omega_0 T)$ of finding $-\hbar/2$. Give a physical interpretation.

c. (This question and the following one involve the concept of a density operator, defined in complement E_{III}. The reader is also advised to refer to complement E_{IV}.) Show that the density matrix ρ_1 of a particle which enters the analyzer is written, in the $\{ | + \rangle, | - \rangle \}$ basis:

$$\rho_1 = \frac{1}{2}\begin{pmatrix} 1 + \cos\theta\cos\omega_0 T & \sin\theta + i\cos\theta\sin\omega_0 T \\ \sin\theta - i\cos\theta\sin\omega_0 T & 1 - \cos\theta\cos\omega_0 T \end{pmatrix}$$

Calculate $\text{Tr}\{\rho_1 S_x\}$, $\text{Tr}\{\rho_1 S_y\}$ and $\text{Tr}\{\rho_1 S_z\}$. Give an interpretation. Does the density operator ρ_1 describe a pure state?

d. Now assume that the speed of an atom is a random variable, and hence the time T is known only to within a certain uncertainty ΔT. In addition, the field B_0 is assumed to be sufficiently strong that $\omega_0 \Delta T \gg 1$. The possible values of the product $\omega_0 T$ are then (modulus 2π) all values included between 0 and 2π, all of which are equally probable.

In this case, what is the density operator ρ_2 of an atom at the moment it enters the analyzer? Does ρ_2 correspond to a pure case? Calculate the quantities $\text{Tr}\{\rho_2 S_x\}$, $\text{Tr}\{\rho_2 S_y\}$ and $\text{Tr}\{\rho_2 S_z\}$. What is your interpretation? In which case does the density operator describe a completely polarized spin? A completely unpolarized spin?

Describe qualitatively the phenomena observed at the analyzer exit when ω_0 varies from zero to a value where the condition $\omega_0 \Delta T \gg 1$ is satisfied.

5. Evolution operator of a spin 1/2 (*cf.* complement F_{III})

Consider a spin 1/2, of magnetic moment $\mathbf{M} = \gamma \mathbf{S}$, placed in a magnetic field $\mathbf{B}_0$ of components $B_x = -\omega_x/\gamma$, $B_y = -\omega_y/\gamma$, $B_z = -\omega_z/\gamma$.
We set:

$$\omega_0 = -\gamma\, |\mathbf{B}_0|$$

a. Show that the evolution operator of this spin is:

$$U(t, 0) = e^{-iMt}$$

where M is the operator:

$$M = \frac{1}{\hbar}\left[\omega_x S_x + \omega_y S_y + \omega_z S_z\right] = \frac{1}{2}\left[\omega_x \sigma_x + \omega_y \sigma_y + \omega_z \sigma_z\right]$$

where σ_x, σ_y and σ_z are the three Pauli matrices (*cf.* complement A_{IV}).

Calculate the matrix which represents M in the $\{ |+\rangle, |-\rangle \}$ basis of eigenvectors of S_z. Show that:

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

b. Put the evolution operator into the form:

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

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

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

and derive the relation:

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

Give a geometrical interpretation.

6. Consider the system composed of two spin 1/2's, $\mathbf{S}_1$ and $\mathbf{S}_2$, and the basis of four vectors $|\pm, \pm\rangle$ defined in complement D_{IV}. The system at time $t = 0$ is in the state

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

a. At time $t = 0$, S_{1z} is measured; what is the probability of finding $-\hbar/2$? What is the state vector after this measurement? If we then measure S_{1x}, what results can be found, and with what probabilities? Answer the same questions for the case where the measurement of S_{1z} yielded $+\hbar/2$.

b. When the system is in the state $|\psi(0)\rangle$ written above, S_{1z} and S_{2z} are measured simultaneously. What is the probability of finding opposite results? Identical results?

c. Instead of performing the preceding measurements, we let the system evolve under the influence of the Hamiltonian:

$$H = \omega_1 S_{1z} + \omega_2 S_{2z}$$

What is the state vector $|\psi(t)\rangle$ at time t? Calculate at time t the mean values $\langle \mathbf{S}_1 \rangle$ and $\langle \mathbf{S}_2 \rangle$. Give a physical interpretation.

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

7. Consider the same system of two spin 1/2's as in the preceding exercise; the state space is spanned by the basis of four states $|\pm, \pm\rangle$.

a. Write the 4×4 matrix representing, in this basis, the S_{1y} operator. What are the eigenvalues and eigenvectors of this matrix?

b. The normalized state of the system is:

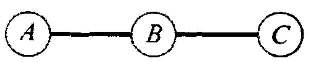
$$|\psi\rangle = \alpha|++\rangle + \beta|+-\rangle + \gamma|-+\rangle + \delta|--\rangle$$

where α, β, γ and δ are given complex coefficients. S_{1x} and S_{2y} are measured simultaneously; what results can be found, and with what probabilities? What happens to these probabilities if $|\psi\rangle$ is a tensor product of a vector of the state space of the first spin and a vector of the state space of the second spin?

c. Same questions for a measurement of S_{1y} and S_{2y}.

d. Instead of performing the preceding measurements, we measure only S_{2y}. Calculate, first from the results of *b* and then from those of *c*, the probability of finding $-\hbar/2$.

8. Consider an electron of a linear triatomic molecule formed by three equidistant atoms. We use $|\varphi_A\rangle$, $|\varphi_B\rangle$, $|\varphi_C\rangle$ to denote three orthonormal states of this electron, corresponding respectively to three wave functions localized about the nuclei of atoms A, B, C. We shall confine ourselves to the subspace of the state space spanned by $|\varphi_A\rangle$, $|\varphi_B\rangle$ and $|\varphi_C\rangle$.



When we neglect the possibility of the electron jumping from one nucleus to another, its energy is described by the Hamiltonian H_0 whose eigenstates are the three states $|\varphi_A\rangle$, $|\varphi_B\rangle$, $|\varphi_C\rangle$ with the same eigenvalue E_0. The coupling between the states $|\varphi_A\rangle$, $|\varphi_B\rangle$, $|\varphi_C\rangle$ is described by an additional Hamiltonian W defined by:

$$W|\varphi_A\rangle = -a|\varphi_B\rangle$$
$$W|\varphi_B\rangle = -a|\varphi_A\rangle - a|\varphi_C\rangle$$
$$W|\varphi_C\rangle = -a|\varphi_B\rangle$$

where a is a real positive constant.

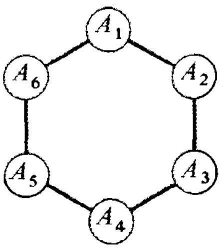
1. Calculate the energies and stationary states of the Hamiltonian $H = H_0 + W$.

2. The electron at time $t = 0$ is in the state $|\varphi_A\rangle$. Discuss qualitatively the localization of the electron at subsequent times t. Are there any values of t for which it is perfectly localized about atom A, B or C?

3. Let D be the observable whose eigenstates are $|\varphi_A\rangle$, $|\varphi_B\rangle$, $|\varphi_C\rangle$ with respective eigenvalues $-d$, 0, d. D is measured at time t; what values can be found, and with what probabilities?

4. When the initial state of the electron is arbitrary, what are the Bohr frequencies that can appear in the evolution of $\langle D\rangle$? Give a physical interpretation of D. What are the frequencies of the electromagnetic waves that can be absorbed or emitted by the molecule?

9. A molecule is composed of six identical atoms A_1, A_2, ... A_6 which form a regular hexagon. Consider an electron which can be localized on each of the atoms. Call $|\varphi_n\rangle$ the state in which it is localized on the nth atom ($n = 1, 2, \ldots 6$). The electron states will be confined to the space spanned by the $|\varphi_n\rangle$, assumed to be orthonormal.



a. Define an operator R by the following relations:

$$R|\varphi_1\rangle = |\varphi_2\rangle;\ R|\varphi_2\rangle = |\varphi_3\rangle;\ \ldots;\ R|\varphi_6\rangle = |\varphi_1\rangle$$

Find the eigenvalues and eigenstates of R. Show that the eigenvectors of R form a basis of the state space.

b. When the possibility of the electron passing from one site to another is neglected, its energy is described by a Hamiltonian H_0 whose eigenstates are the six states $|\varphi_n\rangle$, with the same eigenvalue E_0. As in the previous exercise, we describe the possibility of the electron jumping from one atom to another by adding a perturbation W to the Hamiltonian H_0; W is defined by:

$$W|\varphi_1\rangle = -a|\varphi_6\rangle - a|\varphi_2\rangle; \qquad W|\varphi_2\rangle = -a|\varphi_1\rangle - a|\varphi_3\rangle;$$
$$\ldots\ \ldots; \qquad W|\varphi_6\rangle = -a|\varphi_5\rangle - a|\varphi_1\rangle$$

Show that R commutes with the total Hamiltonian $H = H_0 + W$. From this deduce the eigenstates and eigenvalues of H. In these eigenstates, is the electron localized? Apply these considerations to the benzene molecule.

Exercise 9

Reference: Feynman III (1.2), § 15-4.