Complement B_{IX}

EXERCISES

1. Consider a spin 1/2 particle. Call its spin **S**, its orbital angular momentum **L** and its state vector $| \psi \rangle$. The two functions $\psi_+(\mathbf{r})$ and $\psi_-(\mathbf{r})$ are defined by:

$$\psi_{\pm}(\mathbf{r}) = \langle \mathbf{r}, \pm | \psi \rangle$$

Assume that:

$$\psi_+(\mathbf{r}) = R(r)\left[Y_0^0(\theta, \varphi) + \frac{1}{\sqrt{3}} Y_1^0(\theta, \varphi) \right]$$

$$\psi_-(\mathbf{r}) = \frac{R(r)}{\sqrt{3}} [Y_1^1(\theta, \varphi) - Y_1^0(\theta, \varphi)]$$

where r, θ, φ, are the coordinates of the particle and $R(r)$ is a given function of r.

a. What condition must $R(r)$ satisfy for $| \psi \rangle$ to be normalized?

b. S_z is measured with the particle in the state $| \psi \rangle$. What results can be found, and with what probabilities? Same question for L_z, then for S_x.

c. A measurement of $\mathbf{L}^2$, with the particle in the state $| \psi \rangle$, yielded zero. What state describes the particle just after this measurement? Same question if the measurement of $\mathbf{L}^2$ had given $2\hbar^2$.

2. Consider a spin 1/2 particle. **P** and **S** designate the observables associated with its momentum and its spin. We choose as the basis of the state space the orthonormal basis $| p_x, p_y, p_z, \pm \rangle$ of eigenvectors common to P_x, P_y, P_z and S_z (whose eigenvalues are, respectively, p_x, p_y, p_z and $\pm \hbar/2$).

We intend to solve the eigenvalue equation of the operator A which is defined by:

$$A = \mathbf{S} \cdot \mathbf{P}$$

a. Is A Hermitian?

b. Show that there exists a basis of eigenvectors of A which are also eigenvectors of P_x, P_y, P_z. In the subspace spanned by the kets $| p_x, p_y, p_z, \pm \rangle$, where p_x, p_y, p_z are fixed, what is the matrix representing A?

c. What are the eigenvalues of A, and what is their degree of degeneracy? Find a system of eigenvectors common to A and P_x, P_y, P_z.

3. The Pauli Hamiltonian

The Hamiltonian of an electron of mass m, charge q, spin $\frac{\hbar}{2}\boldsymbol{\sigma}$ (σ_x, σ_y, σ_z : Pauli matrices), placed in an electromagnetic field described by the vector potential $\mathbf{A}(\mathbf{r}, t)$ and the scalar potential $U(\mathbf{r}, t)$, is written:

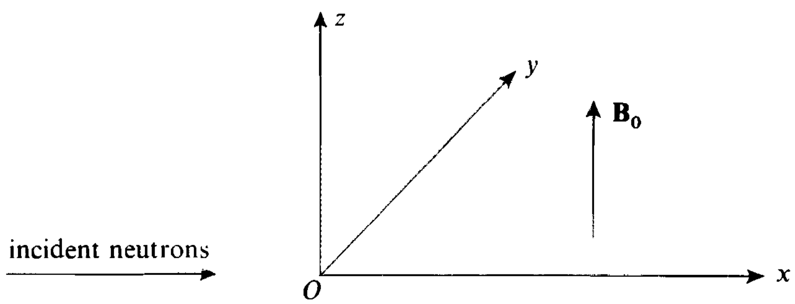
$$H = \frac{1}{2m}[\mathbf{P} - q\mathbf{A}(\mathbf{R}, t)]^2 + qU(\mathbf{R}, t) - \frac{q\hbar}{2m}\boldsymbol{\sigma} . \mathbf{B}(\mathbf{R}, t)$$

The last term represents the interaction between the spin magnetic moment $\frac{q\hbar}{2m}\boldsymbol{\sigma}$ and the magnetic field $\mathbf{B}(\mathbf{R}, t) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{R}, t)$.

Show, using the properties of the Pauli matrices, that this Hamiltonian can also be written in the following form ("the Pauli Hamiltonian"):

$$H = \frac{1}{2m}\{ \boldsymbol{\sigma} . [\mathbf{P} - q\mathbf{A}(\mathbf{R}, t)] \}^2 + qU(\mathbf{R}, t)$$

4. We intend to study the reflection of a monoenergetic neutron beam which is perpendicularly incident on a block of a ferromagnetic material. We call Ox the direction of propagation of the incident beam and yOz the surface of the ferromagnetic material, which fills the entire $x > 0$ region (see figure). Let each incident neutron have an energy E and a mass m. The spin of the neutrons is $s = 1/2$ and their magnetic moment is written $\mathbf{M} = \gamma\mathbf{S}$ (γ is the gyromagnetic ratio and $\mathbf{S}$ is the spin operator).



The potential energy of the neutrons is the sum of two terms:

– the first one corresponds to the interaction with the nucleons of the substance. Phenomenologically, it is represented by a potential $V(x)$, defined by $V(x) = 0$ for $x \leqslant 0$, $V(x) = V_0 > 0$ for $x > 0$.

– the second term corresponds to the interaction of the magnetic moment of each neutron with the internal magnetic field $\mathbf{B}_0$ of the material ($\mathbf{B}_0$ is assumed to be uniform and parallel to Oz). Thus we have $W = 0$ for $x \leqslant 0$, $W = \omega_0 S_z$ for $x > 0$ (with $\omega_0 = -\gamma B_0$). Throughout this exercise we shall confine ourselves to the case:

$$0 < \frac{\hbar\omega_0}{2} < V_0$$

a. Determine the stationary states of the particle which correspond to a positive incident momentum and a spin which is either parallel or antiparallel to Oz.

b. We assume in this question that $V_0 - \hbar\omega_0/2 < E < V_0 + \hbar\omega_0/2$. The incident neutron beam is unpolarized. Calculate the degree of polarization of the reflected beam. Can you imagine an application of this effect?

c. Now consider the general case where E has an arbitrary positive value. The spin of the incident neutrons points in the Ox direction. What is the direction of the spin of the reflected particles (there are three cases, depending on the relative values of E and $V_0 \pm \hbar\omega_0/2$)?

Solution of exercise 4

a. The Hamiltonian H of the particle is:

$$H = \frac{\mathbf{P}^2}{2m} + V(X) + W \tag{1}$$

$V(X)$, which acts only on the orbital variables, commutes with S_z. Since W is proportional to S_z, it also commutes with this operator. Furthermore, $V(X)$ commutes with P_y and P_z, as well as with W (obviously, since W acts only on the spin variables). We can therefore find a basis of eigenvectors common to H, S_z, P_y, P_z, which can be written:

$$| \varphi^{\pm}_{E,p_y,p_z} \rangle = | \varphi^{\pm}_E \rangle \otimes | p_y \rangle \otimes | p_z \rangle \otimes | \pm \rangle \tag{2}$$

with:

$$\begin{aligned} &| \varphi^{\pm}_E \rangle \in \mathscr{E}_x \\ &| p_y \rangle \in \mathscr{E}_y \,;\; P_y | p_y \rangle = p_y | p_y \rangle \\ &| p_z \rangle \in \mathscr{E}_z \,;\; P_z | p_z \rangle = p_z | p_z \rangle \\ &| \pm \rangle \in \mathscr{E}_s \,;\; S_z | \pm \rangle = \pm \frac{\hbar}{2} | \pm \rangle \end{aligned} \tag{3}$$

where the ket $| \varphi^{\pm}_E \rangle$ is a solution of the eigenvalue equation:

$$\left[\frac{P_x^2}{2m} + V(X) + \frac{1}{2m}(p_y^2 + p_z^2) \pm \frac{\hbar\omega_0}{2} \right] | \varphi^{\pm}_E \rangle = E \, | \varphi^{\pm}_E \rangle \tag{4}$$

We assume in the statement of the problem that the neutron beam is normally incident, so we can set $p_y = p_z = 0$. Let $\varphi^{\pm}_E(x) = \langle x | \varphi^{\pm}_E \rangle$ be the wave function associated with $| \varphi^{\pm}_E \rangle$; it satisfies the equation:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \pm \frac{\hbar\omega_0}{2} \right] \varphi^{\pm}_E(x) = E \, \varphi^{\pm}_E(x) \tag{5}$$

Thus the problem is reduced to that of a classical one-dimensional "square well" : reflection from a "potential step" (*cf.* complement H_I).

In the $x < 0$ region, $V(x)$ is zero and the total energy E (which is positive) is greater than the potential energy. We know in this case that the wave function is a superposition of imaginary oscillatory exponentials:

$$\varphi_E^{\pm}(x) = A_{\pm}\, e^{ikx} + B_{\pm}\, e^{-ikx} \qquad \text{if} \quad x < 0 \tag{6}$$

with:

$$k = \sqrt{\frac{2m}{\hbar^2} E} \tag{7}$$

$A_{\pm}$ gives the amplitude of the wave associated with an incident particle having a spin either parallel or antiparallel to Oz. $B_{\pm}$ gives the amplitude of the wave associated with a reflected particle for the same two spin directions.

In the $x > 0$ region, $V(x)$ is equal to V_0 and, depending on the relative values of E and $V_0 \pm \hbar\omega_0/2$, the wave functions can behave like oscillatory or damped exponentials. We shall consider three cases:

(i) If $E > V_0 + \dfrac{\hbar\omega_0}{2}$, we set:

$$k'_{\pm} = \sqrt{\frac{2m}{\hbar^2}\left(E - V_0 \mp \frac{\hbar\omega_0}{2}\right)} \tag{8}$$

and the transmitted wave behaves like an oscillatory exponential:

$$\varphi_E^{\pm}(x) = C_{\pm}\, e^{ik'_{\pm}x} \qquad \text{if} \quad x > 0 \tag{9}$$

Moreover, the continuity conditions for the wave function and its derivative imply [$cf.$ complement H_I, relations (13) and (14)]:

$$\frac{B_{\pm}}{A_{\pm}} = \frac{k - k'_{\pm}}{k + k'_{\pm}} \qquad \frac{C_{\pm}}{A_{\pm}} = \frac{2k}{k + k'_{\pm}} \tag{10}$$

(ii) If, on the other hand, $E < V_0 - \dfrac{\hbar\omega_0}{2}$, we must introduce the quantities $\rho_{\pm}$:

$$\rho_{\pm} = \sqrt{\frac{2m}{\hbar^2}\left(V_0 \pm \frac{\hbar\omega_0}{2} - E\right)} \tag{11}$$

and the wave in the $x > 0$ region is a real, damped exponential (evanescent wave):

$$\varphi_E^{\pm}(x) = D_{\pm}\, e^{-\rho_{\pm}x} \qquad \text{if} \quad x > 0 \tag{12}$$

with, in this case [$cf.$ complement H_I, equations (22) and (23)]:

$$\frac{B_{\pm}}{A_{\pm}} = \frac{k - i\rho_{\pm}}{k + i\rho_{\pm}}\ ; \quad \frac{D_{\pm}}{A_{\pm}} = \frac{2k}{k + i\rho_{\pm}} \tag{13}$$

(iii) Finally, in the intermediate case $V_0 - \dfrac{\hbar\omega_0}{2} < E < V_0 + \dfrac{\hbar\omega_0}{2}$, we have:

$$\varphi_E^{+}(x) = D_{+}\, e^{-\rho_{+}x} \qquad \text{if} \quad x > 0 \tag{14-a}$$

$$\varphi_E^{-}(x) = C_{-}\, e^{ik'_{-}x} \qquad \text{if} \quad x > 0 \tag{14-b}$$

[definitions (8) and (11) of k'_- and ρ_+ are still valid]. Depending on the spin orientation, the wave is either a damped or an oscillatory exponential. We then have:

$$\frac{B_+}{A_+} = \frac{k - i\rho_+}{k + i\rho_+} ; \quad \frac{D_+}{A_+} = \frac{2k}{k + i\rho_+} \tag{15-a}$$

$$\frac{B_-}{A_-} = \frac{k - k'_-}{k + k'_-} ; \quad \frac{C_-}{A_-} = \frac{2k}{k + k'_-} \tag{15-b}$$

b. When $V_0 - \frac{\hbar\omega_0}{2} < E < V_0 + \frac{\hbar\omega_0}{2}$, we are in the situation of case (*iii*) above. If the projection onto Oz of the incident neutron spin is equal to $\hbar/2$, the corresponding reflection coefficient is:

$$R_+ = \left| \frac{B_+}{A_+} \right|^2 = \left| \frac{k - i\rho_+}{k + i\rho_+} \right|^2 = 1 \tag{16}$$

On the other hand, if the projection of the spin onto Oz is equal to $-\hbar/2$, the reflection coefficient is no longer 1, since it is given by:

$$R_- = \left| \frac{B_-}{A_-} \right|^2 = \left(\frac{k - k'_-}{k + k'_-} \right)^2 < 1 \tag{17}$$

Thus we see how the reflected beam can be polarized since, depending on the direction of its spin, the neutron has a different probability of being reflected. An unpolarized incident beam can be considered to be formed of neutrons whose spins have a probability 1/2 of being in the state $| + \rangle$ and a probability 1/2 of being in the state $| - \rangle$. Taking (16) and (17) into account, we see that the probability that a particle of the reflected beam will have its spin in the state $| + \rangle$ is $\frac{1}{1 + R_-}$, while for the state $| - \rangle$ it is $\frac{R_-}{1 + R_-}$. Therefore, the degree of polarization of the reflected beam is:

$$T = \frac{1 - R_-}{1 + R_-} = \frac{2kk'_-}{k^2 + k'^2_-} \tag{18}$$

In practice, reflection from a saturated ferromagnetic substance is actually used in the laboratory to obtain beams of polarized neutrons. To increase the degree of polarization obtained, the beam is made to fall obliquely on the surface of the ferromagnetic mirror; thus, the theoretical results obtained here are not directly applicable. However, the principle of the experiment is the same. The ferromagnetic substance chosen is often cobalt. When cobalt is magnetized to saturation, one can obtain high degrees of polarization T ($T \gtrsim 80\ \%$). Note, furthermore, that the same neutron beam reflection device can serve as an "analyzer" as well as a "polarizer" for spin directions. This possibility has been exploited in precision measurements of the magnetic moment of the neutron.

c. Consider a neutron whose momentum, of magnitude $p = \hbar k$, is parallel to Ox. Assume that the projection $\langle S_x \rangle$ of its spin is equal to $\hbar/2$. Its state is [*cf.* chap. IV, relation (A-20)]:

$$| \psi \rangle = | p \rangle \otimes \frac{1}{\sqrt{2}} [| + \rangle + | - \rangle] \tag{19}$$

with:

$$\langle \mathbf{r} | p \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{ipx/\hbar} \tag{20}$$

How can we construct a stationary state of the particle in which the incident wave has the form (19)? We simply have to consider the state:

$$| \psi_S \rangle = \frac{1}{\sqrt{2}} [| \varphi^+_{E,0,0} \rangle + | \varphi^-_{E,0,0} \rangle] \tag{21}$$

which is a linear combination of two eigenkets of H defined in (2), associated with the same eigenvalue $E = p^2/2m$. The part of the ket $| \psi_S \rangle$ which describes the reflected wave is then:

$$| -p \rangle \otimes \frac{1}{\sqrt{2}} [B_+ | + \rangle + B_- | - \rangle] \tag{22}$$

where B_+ and B_- are given, depending on the case, by (10), (13) or (15) (A_+ and A_- being replaced by 1). Let us calculate, for a state such as (22), the mean value $\langle \mathbf{S} \rangle$. Since this state is a tensor product, the spin variables and the orbital variables are not correlated. Therefore, $\langle \mathbf{S} \rangle$ can easily be obtained from the spin state vector $B_+ | + \rangle + B_- | - \rangle$, which gives:

$$\langle S_x \rangle = \frac{\hbar}{2} \frac{B_+^* B_- + B_-^* B_+}{|B_+|^2 + |B_-|^2} \tag{23-a}$$

$$\langle S_y \rangle = \frac{\hbar}{2} \frac{i(B_-^* B_+ - B_+^* B_-)}{|B_+|^2 + |B_-|^2} \tag{23-b}$$

$$\langle S_z \rangle = \frac{\hbar}{2} \frac{|B_+|^2 - |B_-|^2}{|B_+|^2 + |B_-|^2} \tag{23-c}$$

Three cases can then be distinguished:

(*i*) If $E > V_0 + \hbar\omega_0/2$, we see from (10) that B_+ and B_- are real. Formulas (23) then show that $\langle S_x \rangle$ and $\langle S_z \rangle$ are not zero but that $\langle S_y \rangle = 0$. Upon reflection of the neutron, the spin has thus undergone a rotation about Oy. Physically, it is the difference between the degrees of reflection of neutrons whose spin is parallel to Oz and those whose spin is antiparallel to Oz which explains why the $\langle S_z \rangle$ component becomes positive.

(*ii*) If $E < V_0 - \hbar\omega_0/2$, equations (13) show that B_+ and B_- are not real: they are two complex numbers having different phases but the same modulus. According to (23), we have, in this case, $\langle S_z \rangle = 0$ but $\langle S_x \rangle \neq 0$ and $\langle S_y \rangle \neq 0$. Upon reflection of the neutron, the spin thus undergoes a rotation about Oz. The physical origin of this rotation is the following : because of the existence of the evanescent wave, the neutron spends a certain time in the $x > 0$ region; the Larmor precession about $\mathbf{B}_0$ that it undergoes during this time accounts for the rotation of its spin.

(*iii*) If $V_0 - \hbar\omega_0/2 < E < V_0 + \hbar\omega_0/2$, B_+ is a complex number while B_- is a real number, and their moduli are different. None of the spin components, $\langle S_x \rangle$, $\langle S_y \rangle$ or $\langle S_z \rangle$, is then zero. This rotation of the spin upon reflection of the neutron is explained by a combination of the effects pointed out in (*i*) and (*ii*).