Magnetism in materials

Exercises - Week 01

1. Calculate the magnetic moment of a free electron (with g = 2). What is the Larmor precession frequency of this electron in a magnetic field of flux density 0.3 T? What is the difference in energy of the electron if its spin points parallel or antiparallel to the magnetic field? Convert this energy into a frequency.

2. Let's suppose that we have a magnetic moment $\boldsymbol{\mu}$ in a magnetic $\mathbf{B}$ field. The magnetic $\mathbf{B}$ field is only along the z axis ($\mathbf{B} = B\hat{\mathbf{e}}_z$) and the magnetic moment $\boldsymbol{\mu}$ is initially at an angle of θ to $\mathbf{B}$ and in the xz plane. Found the time dependant expression for $\boldsymbol{\mu}$ and the Larmor frequency (ω_L).

3. Using the definition of spin operators :

$$\hat{S}_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$\hat{S}_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
$$\hat{S}_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

   to prove that :

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hat{S}_z$$

   With all the cyclic permutation (x, y, z) and the two following :

$$\left[\hat{\mathbf{S}}^2, \hat{S}_z\right] = 0$$
$$\hat{\mathbf{S}}^2 \left|\psi\right\rangle = \frac{3}{4}\left|\psi\right\rangle$$

   With $\hat{\mathbf{S}}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$ and $\left|\psi\right\rangle$ an arbitrary state.

4. Prove that :

$$\left[\hat{S}_+, \hat{S}_-\right] = 2\hat{S}_z$$
$$\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+ = 2\left(\hat{S}_x^2 + \hat{S}_y^2\right)$$

   With $\hat{S}_+$ and $\hat{S}_-$ the raising and lowering operator.

5. Using the previous exercise and the following commutation rules

$$\left[\hat{\mathbf{S}}^2, \hat{S}_\pm\right] = 0$$
$$\left[\hat{S}_z, \hat{S}_\pm\right] = \pm\hat{S}_\pm$$

prove that

$$\hat{S}_\pm \left|S, S_z\right\rangle = \sqrt{S(S+1) - S_z(S_z \pm 1)}\left|S, S_z \pm 1\right\rangle$$

Where $|S, S_z\rangle$ represents a state with total spin angular momentum $\hbar^2 S(S+1)$ and z component of spin angular momentum $\hbar S_z$ which is equivalent to say :

$$\hat{\mathbf{S}}^2 \left|S, S_z\right\rangle = S(S+1)\left|S, S_z\right\rangle$$
$$\hat{S}_z \left|S, S_z\right\rangle = S_z \left|S, S_z\right\rangle$$

6. Indicating with $\sigma = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ the Pauli matrices, show that for any $\mathbf{r}$ such that $|\mathbf{r}| = 1$

$$\exp\{i\alpha\mathbf{r}\cdot\sigma\} = \hat{\mathbf{1}}_2 \cos\alpha + i\mathbf{r}\cdot\sigma\sin\alpha$$

7. Using the basis $(|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle)$, it is possible to construct matrix representations of operators such as $\hat{\mathbf{S}}^a \cdot \hat{\mathbf{S}}^b$ remembering that, for example, an operator such as $\hat{S}_z^a$ only operates on the part of the wave function connected with the first spin. Thus we have

$$\hat{S}_z^a = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$
$$\hat{S}_z^b = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Construct similar representations for $\hat{S}_x^a$, $\hat{S}_x^b$, $\hat{S}_y^a$ and $\hat{S}_y^b$ and hence show that

$$\hat{\mathbf{S}}^a \cdot \hat{\mathbf{S}}^b = \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Find the eigenvalues and eigenvectors of this operator.

8. Show that the operator

$$\hat{S}_{\theta,\phi} = \sin\theta\cos\phi\hat{S}_x + \sin\theta\sin\phi\hat{S}_y + \cos\theta\hat{S}_z$$

which represents the spin operator for the component of spin along a direction determined by the spherical polar angles θ and ϕ,has eigenvalue $\pm\frac{1}{2}$ and eigenstates of the form

$$|\uparrow\rangle = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2e^{i\phi} \end{pmatrix}$$
$$|\downarrow\rangle = \begin{pmatrix} \sin\theta/2 \\ -\cos\theta/2e^{i\phi} \end{pmatrix}$$

show further that

$$\hat{S}^2_{\theta\phi} = \frac{1}{4}\hat{\mathbf{1}}_2$$

with $\hat{\mathbf{1}}_2$ the 2×2 identity matrix.

9. If the magnetic field $\mathbf{B}$ is uniform in space, show that this is consistent with writing $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ and show that $\nabla \cdot \mathbf{A} = 0$. Are there other choices of $\mathbf{A}$ that would produce the same $\mathbf{B}$?

10. Using the propriety of the Pauli matrices $\sigma = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$

$$(\sigma \cdot \mathbf{a})(\sigma \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b} + i\sigma \cdot (\mathbf{a} \times \mathbf{b})$$

with $\mathbf{a}, \mathbf{b}$ vectors, show that the kinetic energy operator for an electron $\frac{\hat{\mathbf{p}}^2}{2m}$ can be rewritten as

$$\frac{(\sigma \cdot \hat{\mathbf{p}})^2}{2m}$$

If a magnetic field is applied one must replace $\hat{\mathbf{p}}$ by $\hat{\mathbf{p}} + e\mathbf{A}$ show that this replacement substituted into the previous result leads to kinetic energy of the form

$$\frac{(\hat{\mathbf{p}} + e\mathbf{A})^2}{2m} + g\mu_B \mathbf{B} \cdot \hat{\mathbf{S}}$$

where the g-factor in this case is $g = 2$. (Note: $\hat{\mathbf{p}}$ s an operator and will not commute with $\mathbf{A}$)

11. An electron in a magnetic field aligned along the z-direction has a Hamiltonian (energy) operator

$$\hat{\mathcal{H}} = g\mu_B B \hat{S}_z$$

The time-dependent Schrödinger equation states that

$$\hat{\mathcal{H}}\psi(t) = i\hbar \frac{d\psi}{dt}$$

So that

$$\psi(t) = \exp\{-i\hat{\mathcal{H}}t/\hbar\}\psi(0)$$

Using the result from ex. 6 show that $\psi(t)$ written as a spinor is

$$\psi(t) = \begin{pmatrix} \exp\{-ig\mu_B Bt/2\hbar\} & 0 \\ 0 & \exp\{ig\mu_B Bt/2\hbar\} \end{pmatrix} \psi(0)$$

and using the results from ex. 8 show that this corresponds to the evolution of the spin state in such a way that the expected value of θ is conserved but ϕ rotates with an angular frequency given by $geB/2m$. This demonstrates that the phenomenon of Larmor precession can also be derived from a quantum mechanical treatment.