ENSEMBLE OF ELECTRONS IN MAGNETIC FIELD

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Exercise 14.4.6.

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As an example of a density matrix, we can apply it to an ensemble of spin $\frac{1}{2}$ particles. The density matrix is defined as

$$\rho \equiv \sum_i p_i |i\rangle \langle i| \tag{1}$$

where p_i is the probability of a single system being state $|i\rangle$. For a spin $\frac{1}{2}$ particle, there are only 2 states, so the density matrix can be written as a 2×2 matrix, once we define a basis for the states (for example, the basis of S_z states where $S_z = \pm\frac{\hbar}{2}$). Since any 2×2 matrix can be written as a linear combination of the Pauli matrices and the identity matrix, the density matrix can be written as

$$\rho = a_0 I + \mathbf{A}\cdot\sigma \tag{2}$$

Since the trace of each of the Pauli matrices is zero, and $\mathrm{Tr}I = 2$, we have

$$\mathrm{Tr}\rho = 2a_0 \tag{3}$$

However, we know that $\mathrm{Tr}\rho = 1$, so we must have $a_0 = \frac{1}{2}$, so we can write

$$\rho = \frac{1}{2}(I + \mathbf{a}\cdot\sigma) \tag{4}$$

for some vector **a** whose elements are complex numbers.

To find the average value $\langle\bar{\Omega}\rangle$ of an observable Ω in an ensemble, we can use the density matrix in the form

$$\langle\bar{\Omega}\rangle = \mathrm{Tr}(\Omega\rho) \tag{5}$$

To find $\langle\bar{\sigma}\rangle$, we can work out each component separately. For σ_x we have, using the properties of the σ_i:

$$
\begin{aligned}
\langle\bar{\sigma}_x\rangle &= \mathrm{Tr}\left(\sigma_x\rho\right) &(6)\\
&= \frac{1}{2}\mathrm{Tr}\left(\sigma_x I + a_x\sigma_x^2 + a_y\sigma_x\sigma_y + a_z\sigma_x\sigma_z\right) &(7)\\
&= \frac{1}{2}\mathrm{Tr}\left(\sigma_x + a_x I + ia_y\sigma_z - ia_z\sigma_y\right) &(8)\\
&= \frac{1}{2}\left(0+2a_x+0+0\right) &(9)\\
&= a_x &(10)
\end{aligned}
$$

We can do similar calculations to get the other two components, with the result

$$\langle\bar{\sigma}\rangle = \mathbf{a} \tag{11}$$

Finally, suppose we have an ensemble of electrons in a constant magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$, and that this ensemble is in thermal equilibrium at temperature T. A central result of statistical mechanics (which we haven't covered yet) is that particles in thermal equilibrium obey the Boltzmann distribution, which states that the probability of finding a particle with energy E in the ensemble is

$$p_E \propto e^{-E/kT} \tag{12}$$

where k is the Boltzmann constant. In this case, the energy is that of a magnetic moment μ in a constant magnetic field $\mathbf{B}$, which is

$$H = -\mu\cdot\mathbf{B} = -\gamma\mathbf{S}\cdot\mathbf{B} = -\gamma S_z B \tag{13}$$

There are only two states ($S_z = \pm\frac{\hbar}{2}$), so the probabilities are

$$
\begin{aligned}
p_\uparrow &= \frac{1}{P}e^{\gamma B\hbar/2kT} &(14)\\
p_\downarrow &= \frac{1}{P}e^{-\gamma B\hbar/2kT} &(15)\\
P &= e^{\gamma B\hbar/2kT} + e^{-\gamma B\hbar/2kT} &(16)
\end{aligned}
$$

The density matrix is therefore

$$\rho = \frac{1}{P}\left(e^{\gamma B\hbar/2kT}\left|\uparrow\right\rangle\left\langle\uparrow\right| + e^{-\gamma B\hbar/2kT}\left|\downarrow\right\rangle\left\langle\downarrow\right|\right) \tag{17}$$

In the S_z basis, this is

$$\rho = \frac{1}{P}\left[\begin{array}{cc} e^{\gamma B\hbar/2kT} & 0 \\ 0 & e^{-\gamma B\hbar/2kT} \end{array}\right] \tag{18}$$

We can work out the average magnetic moment for the ensemble as

$$\begin{aligned}
\langle\bar{\mu}\rangle &= \mathrm{Tr}\left(\mu\rho\right) &(19)\\
&= \frac{\hat{\mathbf{z}}}{P}\left[\frac{\gamma\hbar}{2}e^{\gamma B\hbar/2kT} - \frac{\gamma\hbar}{2}e^{-\gamma B\hbar/2kT}\right] &(20)\\
&= \frac{e^{\gamma B\hbar/2kT} - e^{-\gamma B\hbar/2kT}}{e^{\gamma B\hbar/2kT} + e^{-\gamma B\hbar/2kT}}\frac{\gamma\hbar}{2}\hat{\mathbf{z}} &(21)\\
&= \frac{\gamma\hbar}{2}\tanh\frac{\gamma B\hbar}{2kT}\hat{\mathbf{z}} &(22)\\
&= -\frac{e\hbar}{2mc}\tanh\left(-\frac{eB\hbar}{2mckT}\right)\hat{\mathbf{z}} &(23)\\
&= \frac{e\hbar}{2mc}\tanh\frac{eB\hbar}{2mckT}\hat{\mathbf{z}} &(24)
\end{aligned}$$