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WS16/17 Condensed Matter Physics I
Exercise 7. Magnetism -I.

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Notice: *In solving the proposed exercises clearly motivate the passages to reach the result. The use of clear and compact notation is greatly encouraged, as well as the systematic use of dimensional checks of the expressions and results. When you are asked to "evaluate" something this means to provide a numerical evaluation of the expression. In this case, at times, it might be necessary to indicate a parameter whose explicit numerical value is not provided, i.e.* $\omega_c = 1.76\, H$ *(Gauss) Hertz. Otherwise specified, all the evaluations are to be given with 3 significant figures.*

7.1 Diamagnetism of harmonic oscillators… (10 pts)

Let us consider ensemble of N one-dimensional spinless particles of mass m and charge q in a volume V. The particles are in a harmonic potential. Let us disregard mutual interactions between particles.

1. Write the total energy of the system in the ground statel (i.e. at T=0).
   [The total energy of the system in the ground state is
   $$E = N\frac{\hbar\omega}{2}$$
   ]
2. Now evaluate the energy at a finite temperature by applying the appropriate formula $E(T) = \sum_n E_n e^{-\beta E_n} / \sum_n e^{-\beta E_n}$.
   [In this case the thermal average is on all the excited levels $E_n = \hbar\omega\left(\frac{1}{2}+n\right)$:
   $$E(T) = N\frac{\sum_n \hbar\omega\left(\frac{1}{2}+n\right)e^{-\beta\hbar\omega(1/2+n)}}{\sum_n e^{-\beta\hbar\omega(1/2+n)}} = N\frac{\hbar\omega}{2} + \hbar\omega\frac{\sum_n n e^{-\beta\hbar\omega n}}{\sum_n e^{-\beta\hbar\omega n}}.$$
   The geometric series in the denominator can be easiliy summed: $\sum_n e^{-\beta\hbar\omega n} = \frac{1}{1-e^{-\beta\hbar\omega}}$.

Now, the numerator can be mapped into the first derivative of a geometric series with the usual trick:

$$\sum_n n e^{-\beta\hbar\omega n} = -\frac{1}{\hbar\omega}\frac{\partial}{\partial\beta}\sum_n e^{-\beta\hbar\omega n} = \frac{e^{-\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^2}.$$

Therefore we have

$$E(T) = N\hbar\omega\left(\frac{1}{2}+\frac{1}{e^{\beta\hbar\omega}-1}\right).$$

]

3. Consider now a constant magnetic field H applied to the system. Evaluate the energy of the system as a function of the temperature. Which field-dependent term of the one seen in the general theory is not vanishing? Motivate your answer.

[Upon application of a magnetic field H the Hamiltonian aquires the Langevin term. The other therms vanish because the particle is one-dimensional (L=0) and spinless (S=0): For a single particle we have

$$\hat{H} = \hat{T} + \frac{1}{2}m\omega^2\hat{x}^2 + \frac{q^2H^2}{8mc^2}\hat{x}^2$$

This Formally renormalizes the oscillator frequency: $\omega_H = \sqrt{\omega^2 + \frac{q^2H^2}{4m^2c^2}} = \sqrt{\omega^2 + \frac{\omega_c^2}{4}}$. We have introduced here the cyclotron frequency $\omega_c = \frac{qH}{mc}$. Therefore the new energy is simply:

$$E_H(T) = N\hbar\omega_H\left(\frac{1}{2}+\frac{1}{e^{\beta\hbar\omega_H}-1}\right).$$

]

4. Evaluate the total magnetization as a function of temperature, as well as its value and limit behavior for low and high temperatures.

[By derivation we have:

$$M(T) = \frac{\partial E_H(T)}{\partial H} = \frac{\partial\omega_H}{\partial H}\frac{\partial E_H(T)}{\partial\omega_H} = N\hbar\frac{\partial\omega_H}{\partial H}\left[\frac{1}{2}+\frac{1}{e^{\beta\hbar\omega_H}-1} - \frac{\beta\hbar\omega_H e^{\beta\hbar\omega_H}}{(e^{\beta\hbar\omega_H}-1)^2}\right]$$

$$= N\hbar\frac{q^2H}{4m^2c^2}\left[\frac{1}{2\omega_H} + \frac{e^{\beta\hbar\omega_H}(1-\beta\hbar\omega_H)-1}{\omega_H(e^{\beta\hbar\omega_H}-1)^2}\right].$$

]

[Hint: Remember the virial theorem for the harmonic oscillator. In evaluating the thermal average It may be useful to use the harmonic series: if $|a|<1$ $\sum_n a^n = \frac{1}{1-a}$. Moreover, in this particular case the numerator reduces to a particular formal derivative of the numerator.]

7.2 …and of Hydrogen (10 pts)

Consider a gas of Hydrogen atoms of density n=10^{14} cm^{-3}.

1. Show that in the ground state $\langle r^2 \rangle = 3a_0^2$. Remember that the 1s wavefunction is

$$\Psi(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

[The expectation value of the square of the radial is

$$\langle r^2 \rangle = \frac{4\pi}{\pi a_0^3} \int_0^\infty dr\, r^4 e^{-2r/a_0} = \frac{4}{a_0^3} \left(\frac{a_0}{2}\right)^5 \int_0^\infty du\, u^4 e^{-u} = \frac{a_0^2}{8} 4! = 3a_0^2.$$

Here we have used the integral representation of the factorial (Gamma function)

$$\int_0^\infty du\, u^n e^{-u} = \Gamma(n+1) = n!$$

]

2. Calculate the diamagnetic susceptibility in the ground state.

[The diamagnetic susceptibility is the second derivative of the energy with respect to the field. The field-dependent energy term is the Langevin term.

$$E(H) = \frac{e^2 H^2}{8mc^2} \langle x^2 + y^2 \rangle = \frac{e^2 H^2}{8mc^2} \frac{2}{3} \langle r^2 \rangle = \frac{e^2 a_0^2 H^2}{12mc^2}$$

Therefore the susceptibility per atom is

$$\chi_d = -\frac{e^2 a_0^2}{6mc^2}.$$

In atomic Hartree units we have

$$\chi_d = -\frac{1}{6 \times 137^2} = -8.88 \times 10^{-6}\, a_0^3 = -8.88 \times (0.53)^3 \times 10^{-30}\, cm^3$$
$$= -1.32 \times 10^{-30} \frac{cm^3}{atom}.$$

The volume susceptibility is

$$n\chi_d = -1.32 \times 10^{-16}.$$

Compare to a molar susceptibility of about $-7.95 \times 10^{-7}\, cm^3\, mol^{-1}$]

3. Calculate the paramagnetic spin susceptibility at T=100 K.

[

The spin susceptibility per spin is given by the Curie law:

$$\chi_p = \frac{\mu^2}{k_B T}.$$

In atomic units, $k_B T(100\, K) = 3.06 \times 10^{-4}\, Hartree$ and $\mu = e\hbar/2mc = \alpha/2 = 3.6 \times 10^{-3}$ a.u. Therefore

$$\chi_p = \frac{\mu^2}{k_B T} = 1.38 \times 10^{-2}\, a_0^3 = 2.05 \times 10^{-27}\, \frac{cm^3}{atom}.$$

The volume susceptibility is therefore

$$n\chi_p = 2.05 \times 10^{-13}$$

The paramagnetic susceptibility is therefore roughly three order of magnitude larger than the diamagnetic. This is because the diamagnetic term is basically proportional to the area of the average electron orbit (which is treated here like a circular current) and is therefore the smallest among the elements.

NB. The two expressions have the same dimension (cm^3) since $1\, statC = 1\, g^{1/2}\, cm^{3/2}\, s^{-1}$ and $1\, gauss = 1\, statC\, cm^{-2}$.]

4. Does make sense to compare the 0 K diamagnetic susceptibility and the T=100 K paramagnetic susceptibility? Motivate.

   [Yes, because the diamagnetic susceptibility is independent from temperature (only one level!)]

[Hint: use atomics units. Which are the atomic units of the susceptibility?]

7.3 Quantum Paramagnetism (10 pts)

Consider an atom with nonzero magnetic moment in a magnetic field, described by the Hamiltonian

$$\hat{H} = -\mu_B g \hat{J}_z H.$$

Here g is the Lande factor and $\hat{J}_z$ Is the projection of the total angular momentum of the atom along the field direction. Consider the square modulus of the total momentum to be fixed and measured to be in its quantum number J.

1. Find the energy spectrum of the atom.
   [the eigenstates are the momentum eigenstates and the energy spectrum is as follows:
   $$\hat{H}|J, m_J\rangle = -\mu_B g m_J H |J, m_J\rangle.$$
   ]
2. Write down the average magnetic moment of the atom at the temperature T. Present the results in the form $M = \mu B_J(x)$, where x is an appropriate dimensionless parameter. Write down the expression for $B_{1/2}(x)$ and $B_1(x)$.
   [The magnetic moment of the atom in the state $|J, m_J\rangle$ is $\mu_B g m_J$. At temperature T the average magnetic moment is

$$m(T) = \frac{\sum_{m_J=-J}^{J} \mu_B g m_J e^{-\beta\mu_B g m_J H}}{\sum_{m_J=-J}^{J} e^{-\beta\mu_B g m_J H}}$$

The numerator sum can be written as a formal derivative of the denominator:

$$\sum_{m_J=-J}^{J} \mu_B g m_J e^{-\beta\mu_B g m_J H} = -\frac{1}{\beta}\frac{\partial}{\partial H}\sum_{m_J=-J}^{J} e^{-\beta\mu_B g m_J H}.$$

So we can write

$$m(T) = -\frac{1}{\beta}\frac{\partial}{\partial H}\log\sum_{m_J=-J}^{J} e^{-\beta\mu_B g m_J H}$$

The series in the argument can be summed as a geometric series

$$\sum_{m_J=-J}^{J} e^{-\beta\mu_B g m_J H}$$

For J integer:

$$\sum_{m_J=-J}^{J} e^{-\beta\mu_B g m_J H} = 2\cosh(\alpha J/2)\frac{\sinh[\alpha(J+1)/2]}{\sinh[\alpha/2]} - 1$$

For J half-integer:

$$\sum_{m_J=-J}^{J} e^{-\beta\mu_B g m_J H} = 2\cosh(\alpha J/2)\frac{\sinh[\alpha(2J+1)/4]}{\sinh[\alpha/4]} - 2$$

Here $\alpha = \beta\mu_B g H$.

Now $\frac{\partial}{\partial H} = \beta\mu_B g\frac{\partial}{\partial\alpha}$, and $\frac{\partial}{\partial\alpha}\log f(\alpha) = \frac{1}{f(\alpha)}\frac{\partial f}{\partial\alpha}$ the rest is calculation.]

3. Now consider J integer and sum the geometric series and obtain an explicit form for B. Compare the sum for J=1/2 with the result obtained in the preceeding point. Are they the same?

4. Find the magnetic susceptibility per atom.

[Hint: es $\sum_{n=0}^{N} a^n = \frac{1-a^{N+1}}{1-a}$.]