HW#2 Solutions, Chapter 8, Problems 1-5

1. Diamagnetic susceptibility of atomic hydrogen:

Wave function $\psi = \dfrac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$. $a_0 = 0.529\,\mathring{A}$. The appropriate expression for atomic diamagnetic susceptibility is:

$$\chi_m \equiv \frac{\vec{M}}{\vec{H}} = \frac{n\,|\langle \vec{m} \rangle|}{|\vec{B}|/\mu_0} = -\frac{\mu_0 n e^2}{6 m_e} < r >^2$$

where n is the number of atoms N per unit volume V.

$$< r^2 > = < \psi_0 \left| r^2 \right| \psi_0 > = \frac{1}{\pi a_0^3} \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} e^{-r/a_0} r^2 e^{-r/a_0} r^2 \sin\theta dr d\theta d\phi$$

can immediately integrate over θ and φ to get

$$< r^2 > = \frac{4}{a_0^3} \int_0^{\infty} r^4 e^{-2r/a_0} dr ......\{ let\ u = 2r/a_0,\ du = 2dr/a_0\ .$$

$$< r^2 > = \frac{4}{a_0^3} \left(\frac{a_0}{2} \right) \int_0^{\infty} u^4 e^{-u} du = a_0^2 \frac{4(4!)}{2^5} = 3a_0^2$$

$$\chi = \frac{-n\mu_0 \left(1.6\times10^{-19}\right)^2 \cdot 3\left(0.53\times10^{-10}\right)^2}{6\left(9.11\times10^{-31}\right)} = -\frac{N}{V}\left(5.0\times10^{-35}\right) = [MKSA]$$

Let N = Avogadro's number $= 6.02\times10^{23}\ atoms/mole$.

$$\Rightarrow \chi = -3.0\times10^{-11}/V$$ where V is the volume of the 1-mole sample in m^3.

2. Paramagnetic Problem: (a) For any magnetic dipole $U = -\vec{m}\cdot\vec{B}$, and for a total angular momentum $\vec{J}$, $\vec{m} = -g\mu_B\vec{J}$ where g = 1 and thus $-\vec{m}\cdot\vec{B} = g\mu_B\vec{J}\cdot\vec{B} = \mu_B m_J \cdot B$ where $m_J = +1, 0, and -1$ for J=1. So we have three energy levels $U_1 = \mu_B B$, $U_2 = 0, U_3 = -\mu_B B$

(b) according to Boltzmann statistics $<\vec{m}>= N\cdot\sum_{n=1}^{3}\vec{m}_n e^{-U_n/k_BT}$, $N=(e^{-\mu_B B/k_BT}+1+e^{\mu_B B/k_BT})^{-1}$, So

along z axis, $\vec{m}_1=-\mu_B\hat{z};\vec{m}_2\equiv 0;\vec{m}_3=+\mu_B\hat{z}$

and $$<\vec{m}>= N\mu_B\cdot\hat{z}(-e^{-\mu_B B/k_BT}+e^{\mu_B B/k_BT})$$

(c) $\vec{M}=\chi_m \vec{B}/\mu_o \Rightarrow \chi_m=\mu_o|\vec{M}|/|\vec{B}|=\mu_o n|<\vec{m}>|/|\vec{B}|$ where n is the density of magnetic dipoles per unit volume so for $\vec{B}$ along $\hat{z}$, $\chi_m=(\mu_o\mu_B n\cdot N/B)(e^{\mu_B B/k_BT}-e^{-\mu_B B/k_BT})$

(d) For high temperatures, $\mu_B B/k_BT\ll 1\Rightarrow \chi_m\approx \mu_0\mu_B nN2\mu_B B/(k_BT)$ (by Taylor expansion)

But at high temperatures: $N=(e^{-\mu_B B/k_BT}+1+e^{\mu_B B/k_BT})^{-1}\approx 1/3$ (also by Taylor expansion)

so $\chi_m\cong 2n\mu_o\mu_B{}^2/3k_BT\equiv C/T\Rightarrow C=2\cdot n\mu_o\mu_B{}^2/3k_B$

(e) for $n=1x10^{23}[cm^{-3}]=1x10^{29}[m^{-3}]\Rightarrow \chi_m=C/T=0.522/T=1.74x10^{-3}$ at T = 300 K.

3. Langevin model of Paramagnetism

(a) For the classical magnetic dipole, we have $\boldsymbol{U_m}=-\vec{\boldsymbol{m}}_0\cdot\vec{\boldsymbol{B}}_{\boldsymbol{local}}$. Without loss of generality we can choose B_{local} (henceforth written as B_L) along the z axis in a spherical coordinate system, so that $U_m = -m_0B_L\cos\theta$. The probability phase space is defined simply by the solid angle since the dipole can be pointed anywhere along a direction θ,ϕ . The probability of pointing in a certain direction is dictated by the Boltzmann ansatz,

$$\boldsymbol{f}(\boldsymbol{\theta},\boldsymbol{\phi})=\frac{\exp[-\boldsymbol{U}(\boldsymbol{\theta},\boldsymbol{\phi})/\boldsymbol{k_BT})]}{\int_0^{4\pi}\exp[-\boldsymbol{U}(\boldsymbol{\theta},\boldsymbol{\phi})/\boldsymbol{k_BT}]\boldsymbol{d}\Omega}=\frac{\exp[\boldsymbol{m}_0\boldsymbol{B_L}\cos\boldsymbol{\theta}/\boldsymbol{k_BT})]}{\int_0^{4\pi}\exp[\boldsymbol{m}_0\boldsymbol{B_L}\cos\boldsymbol{\theta}/\boldsymbol{k_BT}]\boldsymbol{d}\Omega}$$

where dΩ is the differential solid angle, dΩ = sinθ dθ dϕ.. It also allows us to treat the dipole using the inherently random radial unit vector in spherical coordinates,

$$\vec{m} = m_0\hat{r} = m_0(\hat{x}\sin\theta\cos\varphi + \hat{y}\sin\theta\sin\varphi + \hat{z}\cos\theta)$$

This by statistical principles, we can write the mean value of the magnetic dipole moment:

$$<\vec{m}>= \frac{\int_0^{2\pi}\int_0^{\pi} m_0(\hat{x}\sin\theta\cos\varphi + \hat{y}\sin\theta\sin\varphi + \hat{z}\cos\theta)\exp[m_0 B_L\cos\theta)/k_B T]\sin\theta d\theta d\phi}{\int_0^{2\pi}\int_0^{\pi}\exp[m_0 B_L\cos\theta/k_B T]\sin\theta d\theta d\phi}$$

Clearly the terms in the numerator that include the x and y unit vectors vanish since they involve integrating cosϕ or sinϕ from 0 to 2π. The term containing the z unit vector can be evaluated through the substitution $W = m_0B_L/k_BT$.

$$<\vec{m}>= \frac{\int_0^{\pi} m_0(\hat{z}\cos\theta)\exp[W\cos\theta]\sin\theta d\theta}{\int_0^{\pi}\exp[W\cos\theta]\sin\theta d\theta} \qquad (1)$$

Evaluation of the denominator leads to

$$\int_0^{\pi}\exp[W\cos\theta]\sin\theta d\theta = -\left.\frac{\exp(W\cos\theta)}{W}\right|_0^{\pi} = \frac{2}{W}\sinh W \qquad (2)$$

The numerator is a bit more work, requiring integration by parts. We set U = cosθ dθ and dV = sinθexp(Wcosθ), and get dU = -sinθdθ and V = -exp(Wcosθ)/W

$$\int_0^{\pi} m_0(\hat{z}\cos\theta)\exp[W\cos\theta]\sin\theta d\theta d\phi = UV\big|_0^{\pi} - \int_0^{\pi} VdU$$

$$U\cdot V\big|_0^{\pi} = \left.\frac{-\cos\theta}{W}\exp(W\cos\theta)\right|_0^{\pi} = \frac{e^{-W}}{W} + \frac{e^{W}}{W} = \frac{2}{W}\cosh W \qquad (3)$$

and $$-\int_0^{\pi} VdU = -\int_0^{\pi}\frac{\sin\theta}{W}\exp(W\cos\theta)d\theta = \left.\frac{\exp(W\cos\theta)}{W^2}\right|_0^{\pi} = \frac{e^{-W}}{W^2} - \frac{e^{W}}{W^2} = \frac{-2\sinh W}{W^2} \qquad (4)$$

Summing (3) and (4), dividing by (2), and substitution into (1) yields

$$<\vec{\boldsymbol{m}}>=\frac{\boldsymbol{m}_0\hat{\boldsymbol{z}}[(2/\boldsymbol{W})\cosh\boldsymbol{W}-(2/\boldsymbol{W}^2)\sinh\boldsymbol{W}}{(2/\boldsymbol{W})\sinh\boldsymbol{W}}=\boldsymbol{m}_0\hat{\boldsymbol{z}}[\coth\boldsymbol{W}-(1/\boldsymbol{W})]$$

$$<\vec{\boldsymbol{m}}>=\boldsymbol{m}_0\hat{\boldsymbol{z}}[\coth(\boldsymbol{m}_0\boldsymbol{B_L}/\boldsymbol{k_B T})-(\boldsymbol{k_B T}/\boldsymbol{m}_0\boldsymbol{B_L})]$$

This is the famous Langevin function

(b) If there are n such dipoles per unit volume, the mean magnetization becomes

$$<\vec{\boldsymbol{M}}>=\boldsymbol{n}<\vec{\boldsymbol{m}}>=\boldsymbol{n}\cdot\boldsymbol{m}_0\hat{\boldsymbol{z}}[\coth(\boldsymbol{m}_0\boldsymbol{B_L}/\boldsymbol{k_B T})-(\boldsymbol{k_B T}/\boldsymbol{m}_0\boldsymbol{B_L})] \qquad (5)$$

In the limit of high temperature, it is easy to show that the Taylor's series of coth(x) for small x is

$$\coth(x) = 1/x + x/3 + \ldots.$$

The first term of this cancels the last term in (5), so that

$$<\vec{\boldsymbol{M}}>\approx\boldsymbol{n}\cdot\boldsymbol{m}_0\left(\frac{\boldsymbol{m}_0\boldsymbol{B_L}}{\boldsymbol{k_B T}}\right)\hat{\boldsymbol{z}}$$

The high temperature limit of the paramagnetic susceptibility is

$$\chi_m\equiv\frac{|\vec{\boldsymbol{M}}|}{|\vec{\boldsymbol{H}}|}=\frac{|\vec{\boldsymbol{M}}|}{|\vec{\boldsymbol{B}}|/\mu_0|}=\left(\frac{\boldsymbol{n}\boldsymbol{m}_0^2\mu_0}{\boldsymbol{k_B T}}\right)$$

4. Another Paramagnetic Problem: (a) For any magnetic dipole $U=-\vec{m}\cdot\vec{B}$, and for a total angular momentum $\vec{J}$, $\vec{m}=-g\mu_B\vec{J}$ where g = 1. Thus $-\vec{m}\cdot\vec{B}=g\mu_B\vec{J}\cdot\vec{B}=\mu_B m_J\cdot B$ where $m_J=+3/2,+1/2,-1/2,-3/2$ for J=3/2. So there are *four energy levels* $U_1=3\mu_B B/2$, $U_2=\mu_B B/2$ $U_3=-\mu_B B/2$ $U_4=-3\mu_B B/2$

(b) occupancy probability $f_n = Ne^{-U_n/k_BT}$,

$$N=(e^{-3\mu_B B/2k_BT}+e^{-\mu_B B/2k_BT}+e^{\mu_B B/2k_BT}+e^{3\mu_B B/2k_BT})^{-1}$$

(c) average magnetic dipole $<\vec{m}>=N\cdot\sum_{n=1}^{4}\vec{m}_n e^{-U_n/k_BT}$. So along z axis (direction of B field),

$\vec{m}_1=-3\mu_B\hat{z}/2;\vec{m}_2=-\mu_B\hat{z}/2;\vec{m}_3=\mu_B\hat{z}/2;\vec{m}_4=3\mu_B\hat{z}/2$ and

$$<\vec{m}>=N\mu_B\cdot\hat{z}[-(3/2)e^{-3\mu_B B/2k_BT}-(1/2)e^{-\mu_B B/2k_BT}+(1/2)e^{\mu_B B/2k_BT}+(3/2)e^{3\mu_B B/2k_BT}]$$

(d) $\vec{M}=\chi_m\vec{B}/\mu_o\Rightarrow\chi_m=\mu_o|\vec{M}|/|\vec{B}|=\mu_o n|<\vec{m}>|/|\vec{B}|$ where n is the density of magnetic dipoles,so

$$\chi_m = (\mu_o \mu_B n \cdot N / B)[(3/2)e^{3\mu_B B/2k_B T} + (1/2)e^{\mu_B B/2k_B T} - (1/2)e^{-\mu_B B/2k_B T} - (3/2)e^{-3\mu_B B/2k_B T}]$$

(e) For high temperature, $N = (e^{-3\mu_B B/2k_B T} + e^{-\mu_B B/2k_B T} + e^{\mu_B B/2k_B T} + e^{3\mu_B B/2k_B T})^{-1} \approx 1/4$.

But $$-(3/2)e^{-3\mu_B B/2k_B T} - (1/2)e^{-\mu_B B/2k_B T} + (1/2)e^{\mu_B B/2k_B T} + (3/2)e^{3\mu_B B/2k_B T}$$

$$\approx -(\frac{3}{2})[1 - \frac{3\mu_B B}{2k_B T}] - (\frac{1}{2})[1 - \frac{\mu_B B}{2k_B T}] + (\frac{1}{2})[1 + \frac{\mu_B B}{2k_B T}] + (\frac{3}{2})[1 + \frac{3\mu_B B}{2k_B T}] = \frac{20\mu_B B}{4k_B T}$$

so that $\chi_m \approx (5/4)(\mu_o \mu_B^2 n / k_B T) \equiv C/T$, and yes, it can be written as $\chi_m = C/T$

(f) We know from the Heisenberg model of ferromagnetism that the factor g is very large of order 1000. This is caused by spin-spin interaction, also called the "exchange" interaction.

5. **Curie-Weiss-Heisenberg Model of Ferromagnetism**

(a) If $\vec{B}_{local} = \vec{B}_{in} + \gamma\mu_0 \vec{M}$, then by inserting (5) from above, we can write

$$\vec{B}_{local} \equiv \vec{B}_L = \vec{B}_{in} + \gamma\mu_0 n\vec{m} = \vec{B}_{in} + \gamma\mu_0 n \cdot m_0 \hat{z}[\coth(m_0 B_L / k_B T) - (k_B T / m_0 B_L)] \quad (6)$$

This can be re-written as

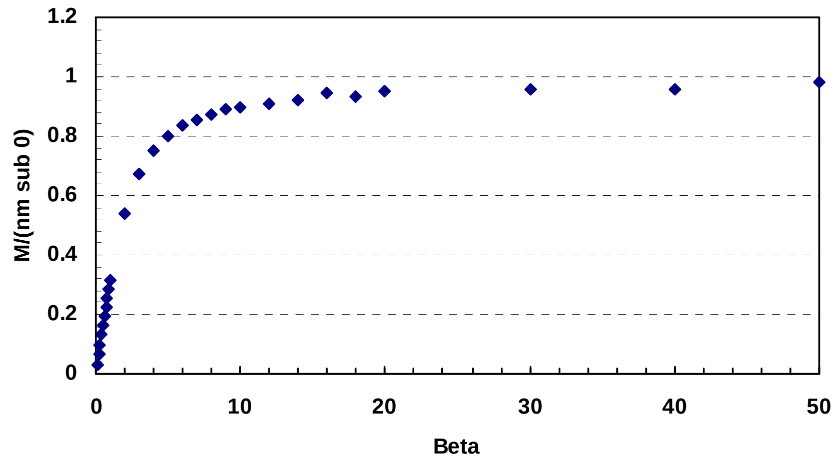
$$B_L = B_{in} + \gamma\mu_0 n \cdot m_0 [\coth(m_0 B_L / k_B T) - (k_B T / m_0 B_L)] \quad (7)$$

since B_L and B_{in} are both along the z axis. Eqn (7) is an *implicit* equation in B_L since B_L occurs on both sides and can not be isolated.

(b) Eqn (7) can be solved uniquely for B_L in the case of spontaneous magnetization, which means that $B_L \neq 0$ even when $B_{in} = 0$. From such a solution, we can get M through $M = B_L/(\gamma\mu_0)$. To proceed we re-write (7) using $\beta = m_0 B_L / k_B T$, under the spontaneous condition:

$$k_B T \beta / m_0 = \gamma\mu_0 n \cdot m_0 [\coth(\beta) - (1/\beta)]$$

or
$$k_B T \beta / (n\gamma\mu_0 m_0^2) \equiv \alpha \cdot \beta = [\coth(\beta) - (1/\beta)] \quad (8)$$



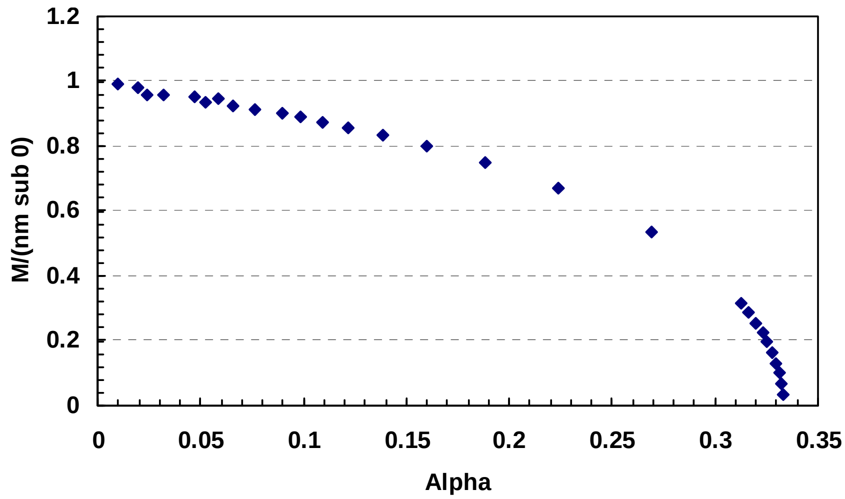


Fig. 2. Top: Magnetization vs β. Bottom: Normalized magnetization vs α, a quantity proportional to temperature. This is the characteristic ferromagnetic phase transition curve. The value of alpha where M reaches zero defines the Curie temperature.

therefore, an atomic concentration of 2/(2.87 Ang) ... And we assume there is one magnetic moment per atom. Thus, if $m_0 = \mu_B = 9.27\times10^{-24}$ [MKSA], and we set $T_C = 300$ K, we can solve for $\gamma = 1355$, which is not much higher than expected. Putting in a more realistic value of m_0 would decrease this quadratically as seen from (10) above

Solution table

β	α
0.1	0.333
0.2	0.332
0.3	0.331
0.4	0.33
0.5	0.328
0.6	0.325

0.7	0.323
0.8	0.32
0.9	0.3165
1	0.313
2	0.269
3	0.224
4	0.188
5	0.16
6	0.139
7	0.122
8	0.109
9	0.0987
10	0.09
12	0.076
14	0.066
16	0.059
18	0.052
20	0.0475
30	0.032
40	0.024
50	0.0196
100	0.0099