Ex5716: Ferromagnetism for Cubic Crystal

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The Problem:

A cubic crystal which exhibits ferromagnetism at low temperature, can be described near the critical temperature T_c by an expansion of a Gibbs free energy

$$G(\mathbf{H}, T) = G_0 + \frac{1}{2} r\mathbf{M}^2 + u\mathbf{M}^4 + v\sum_{i=1}^{3} M_i^4 - \mathbf{H}\cdot\mathbf{M} \tag{1}$$

where $\mathbf{H} = (H_1, H_2, H_3)$ is the external field and $\mathbf{M} = (M_1, M_2, M_3)$ is the total magnetization; $r = a\,(T - Tc)$ and G_0, a, u and v are independent of $\mathbf{H}$ and $T, a > 0, u > 0$. The constant v is called the cubic anisotropy and can be either positive or negative.

(a) At $\mathbf{H} = 0$, find the possible solutions of $\mathbf{M}$ which minimize G and the corresponding values of $G\,(0, T)$ (these solutions are characterized by the magnitude and direction of $\mathbf{M}$. Show that the region of stability of G is $u + v > 0$ and determine the stable equilibrium phases when $T < T_c$ for the cases (i) $v > 0$, (ii) $-u < v < 0$.

(b) Show that there is a second order phase transition at $T = T_c$, and determine the critical indices α, β and γ for this transition, i.e. $C_{V,H=0} \sim |T - T_c|^{-\alpha}$ for both $T > T_c$ and $T < T_c$, $|\mathbf{M}|_{H=0} \sim (Tc - T)^{\beta}$ for $T < T_c$ and $\chi_{ij} = \partial M_i/\partial H_j \sim \ \delta_{ij}|T - T_c|^{-\gamma}$ for $T > T_c$.

The solution:

(a) For $\mathbf{H} = 0$ and $\mathbf{M} = \sqrt{M_1^2 + M_2^2 + M_3^2}$ one can find $\mathbf{M}$ which minimizes Gibbs free energy by applying a gradient in $\mathbf{M}$

$$\vec{\nabla}_{\mathbf{M}} G(0, T) = \sum_i \hat{i}\frac{\partial}{\partial M_i} G(0, T) = \sum_i \hat{i}(rM_i + 4uM_i\mathbf{M}^2 + 4vM_i^3) = \sum_i \hat{i}M_i(r + 4u\mathbf{M}^2 + 4vM_i^2) \tag{2}$$

Where $i = 1, 2, 3$ and the corresponding directions.

For stability, we demand that $G \to \infty$ as each $M_i \to \pm\infty$. Because each M_i is independent and from symmetry considerations, we can check what happens to G by taking the limit in each direction separately. It would be easier to see that for each M_i , $\vec{\nabla}_M G$ will give an increasing monotonic function* as $M_i \to \infty$.

$$\lim_{M_i\to\infty} \vec{\nabla}_{\mathbf{M}} G(0, T) = \lim_{M_i\to\infty} \sum_i \hat{i}M_i(r + 4u\mathbf{M}^2 + 4vM_i^2) \tag{3}$$

A polynomial function at infinity governed by the highest power of the polynomial function. therefore

$$\lim_{M_i\to\infty} \vec{\nabla}_{\mathbf{M}} G(0, T) \to \lim_{M_i\to\infty} 4(u + v)M_i^3 > 0 \tag{4}$$

The latter requires $u + v > 0$, so this is the stability region of G.

* From symmetry decreasing monotonic function as each $M_i \to -\infty$ requires the same condition

In order to find the extrema points, we may require $\vec{\nabla}_{\mathbf{M}} G(0,T) = 0$, meaning each direction must equal 0 separately. We can find solutions in different cases which are distinct by the number of non-zero components of the magnetization vector.
The trivial solution is $M_i = 0$ for every $\hat{i}$ direction.
Next let's choose two of the magnetization components to be zero $M_i, M_j = 0$ and one non-zero $M_k \neq 0$. This will leave us with the equation

$$r + 4(u+v)M_k^2 = 0 \rightarrow M_k^2 = \frac{-r}{4(u+v)} \tag{5}$$

Where i, j, k can be any permutation of $1, 2, 3$.
Another option for solution is $M_i = 0$ and $M_j, M_k \neq 0$ and we have 2 coupled equations

$$\begin{aligned} &r + 4(u+v)M_j^2 + 4uM_k^2 = 0 \\ &r + 4(u+v)M_k^2 + 4uM_j^2 = 0 \end{aligned} \tag{6}$$

or in matrices form

$$-\frac{r}{4}\begin{pmatrix}1\\1\end{pmatrix} = \begin{pmatrix} u+v & u \\ u & u+v \end{pmatrix}\begin{pmatrix} M_j^2 \\ M_k^2 \end{pmatrix} \tag{7}$$

Leading to the solution $M_j^2 = M_k^2 = \frac{-r}{4(2u+v)}$. The last option is 3 non-zero components $M_i, M_j, M_k \neq 0$ leading to the matrix equation

$$-\frac{r}{4}\begin{pmatrix}1\\1\\1\end{pmatrix} = \begin{pmatrix} u+v & u & u \\ u & u+v & u \\ u & u & u+v \end{pmatrix}\begin{pmatrix} M_i^2 \\ M_j^2 \\ M_k^2 \end{pmatrix} \tag{8}$$

and its solution $M_{i,j,k}^2 = \frac{-r}{4(3u+v)}$.
So we have the possible extrema points for (M_i^2, M_j^2, M_k^2)

$$(0,0,0), (0,0,\frac{-r}{4(u+v)}), (0, \frac{-r}{4(2u+v)}, \frac{-r}{4(2u+v)}), (\frac{-r}{4(3u+v)}, \frac{-r}{4(3u+v)}, \frac{-r}{4(3u+v)}) \tag{9}$$

in any permutation of 1,2,3.
Since this is the solution for the quadratic components of the extrema point of the magnetization, we can see that in the case of $r > 0$ the last 3 solutions for the magnetization are non-physical, leaving the trivial solution the only physical solution.

Next, we want to check the stability of the solution (if it's a minimum), so we calculate the Hessian matrix

$$\begin{pmatrix} r + 4u\mathbf{M}^2 + (12v+8u)M_x^2 & 8uM_xM_y & 8uM_xM_z \\ 8uM_yM_x & r + 4u\mathbf{M}^2 + (12v+8u)M_y^2 & 8uM_yM_z \\ 8uM_zM_x & 8uM_zM_y & r + 4u\mathbf{M}^2 + (12v+8u)M_z^2 \end{pmatrix} \tag{10}$$

Due to the symmetry in this problem and since the solution found above is for quadratic components M_i^2, if (M_1, M_2, M_3) is a solution then any permutation of $(\pm M_1, \pm M_2, \pm M_3)$ is also a solution.
We can map all the degenerate solutions of (M_i, M_j, M_k) to the corresponding eigenvalues of the Hessian

Magnetization Vector	Eigenvalues of the Hessian
$\mathbf{M^{(1)}} = \left(\pm\sqrt{\frac{-r}{4(3u+v)}}, \pm\sqrt{\frac{-r}{4(3u+v)}}, \pm\sqrt{\frac{-r}{4(3u+v)}}\right)$	$-2r, -\frac{2rv}{3u+v}, -\frac{2rv}{3u+v}$
$\mathbf{M^{(2)}} = \left(\pm\sqrt{\frac{-r}{4(2u+v)}}, \pm\sqrt{\frac{-r}{4(2u+v)}}, 0\right)$	$-\frac{2rv}{2u+v}, \frac{rv}{2u+v}, -2r$
$\mathbf{M^{(3)}} = \left(\pm\sqrt{\frac{-r}{4(u+v)}}, 0, 0\right)$	$\frac{rv}{u+v}, \frac{rv}{u+v}, -2r$
$\mathbf{M^{(4)}} = \left(0,0,0\right)$	r, r, r

As we could predict, the trivial solution $\mathbf{M^{(4)}}$ is unstable point for $r < 0$. We can also say that $\mathbf{M^{(2)}}$ is always unstable since its first two eigenvalues of the Hessian must have opposite signs.

Now let us determine the stable equilibrium phases for $T < T_c$ (meaning $r < 0$) and
(i) $v > 0$
In this case the eigenvalues of the Hessian of $\mathbf{M^{(1)}}$ are all positive, and some of the eigenvalues of the Hessian of $\mathbf{M^{(3)}}$ are negative, meaning these are saddle points. In this case, the corresponding value of the Gibbs free energy at the stable points is $G(0,T) = G_0 - \frac{9r^2}{16(3u+v)}$
(ii) $-u < v < 0$
In this case the eigenvalues of the Hessian of $\mathbf{M^{(3)}}$ are all positive, and some of the eigenvalues of the Hessian of $\mathbf{M^{(1)}}$ are negative, meaning these are saddle points. In this case, the corresponding values of the Gibbs free energy at the stable points is $G(0,T) = G_0 - \frac{3r^2}{16(u+v)}$

(b)
Second order transition is defined by continuity of magnetization at stable equilibrium phase (which is the order parameter of the system) as a function of the temperature and a discontinuity in the derivative at $T = T_c$.
With that in mind we see that for $T > T_c$, $M = 0$ and for $T < T_c$,$M \propto \sqrt{-r} = \sqrt{a(T_c - T)}$.
For $T \to T_c$, $\sqrt{-r} \to 0$ which gives us the continuity at T_c for $M(T)$, while $\frac{\partial M}{\partial T}(T) \propto \frac{1}{\sqrt{-r}}$ for $T < T_c$ and $\frac{\partial M}{\partial T}(T) = 0$ for $T > T_c$ which gives us the discontinuity in the derivative at $T = T_c$, and as expected, a second order phase transition.

We want to find the critical indices. The index α is defined by $C_{V,H=0} \sim |T - T_c|^{-\alpha}$ for both $T > T_c$ and $T < T_c$.

$$C_{V,H=0} = -T\frac{\partial^2 G(T, H = 0)}{\partial T^2} = -T\frac{\partial}{\partial T}(\vec{\nabla}_{\mathbf{M}} G(T, H = 0)\frac{\partial M}{\partial T}) \tag{11}$$

For $T > T_c$, $G(T, H = 0) = G_0$ so the heat capacity is $C_{V,H=0} = 0$ and index $\alpha = 0$ in that case.
For $T < T_c$, $|\mathbf{M}| \propto \sqrt{-r} \sim \sqrt{T_c - T}$ so $\frac{\partial M}{\partial T} \propto -\frac{1}{2\sqrt{T_c - T}}$.

$$C_{V,H=0} \sim -T\frac{\partial}{\partial T}(M_i(r + 4u\mathbf{M} + 4vM_i^2)\frac{\partial M}{\partial T}) \tag{12}$$

and for T around T_c we can take only the first order in M_i

$$C_{V,H=0} \sim -T\frac{\partial}{\partial T}(rM_i(-\frac{1}{2\sqrt{T_c - T}})) \sim -T\frac{\partial}{\partial T}(r) \sim T_c \tag{13}$$

which means $\alpha = 0$.
The index β is defined by $|\mathbf{M}|_{H=0} \sim (T_c - T)^\beta$ for $T < T_c$. In both cases for stable phases for $r < 0$ in the previous section the magnitude of the magnetization is

$$|\mathbf{M}|_{H=0} \propto \sqrt{-r} = \sqrt{T_c - T} = (T_c - T)^{\frac{1}{2}} \tag{14}$$

meaning $\beta = \frac{1}{2}$.

The index γ is defined by $\chi_{ij} = \partial M_i/\partial H_j \sim \delta_{ij}|T - T_c|^{-\gamma}$ for $T > T_c$. In order to find the index, we need to calculate the gradient of the Gibbs free energy again for $\mathbf{H} \neq 0$ and find the magnetization that minimize it.

$$\vec{\nabla}_{\mathbf{M}} G(0,T) = \sum_i \hat{i}M_i(r + 4u\mathbf{M}^2 + 4vM_i^2) - H_i = 0 \tag{15}$$

We get a vector equation, and for each direction

$$M_i(r + 4u\mathbf{M}^2 + 4vM_i^2) = H_i \tag{16}$$

For $T > T_c$ and weak magnetic field $\mathbf{H}$ we know that $M_i \to 0$, so we can take the first order of M_i

$$H_i \approx M_i r \to M_i \approx \frac{1}{r} H_i \tag{17}$$

and the susceptibility

$$\chi_{ij} = \partial M_i / \partial H_j \approx \frac{1}{r} \frac{\partial H_i}{\partial H_j} \sim \delta_{ij}(T - T_c)^{-1} \tag{18}$$

meaning $\gamma = 1$.