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Problem Set 9

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M1-S2 2021—2022

Exercise 1 : Crystalline anisotropy energy

Iron crystals have cubic symmetry. The directions of easy magnetization of an iron crystal are the crystalline directions [100], [010], and [001]. We denote α, β, and γ the directional cosines of the magnetization with respect to these directions (the directional cosine of a vector is the cosine of the angle between the vector and the direction). The energy density of crystalline anisotropy is expanded in a power series of these cosines as

$$W(\alpha,\beta,\gamma) = \sum_{p,q,r} A_{p,q,r}\alpha^p\beta^q\gamma^r,$$

where the sum is running over integers $p, q, r \geq 0$. In the case of iron, the crystal symmetry allows to simplify the general expression.

It is equivalent to

$$\frac{\vec{M}}{|\vec{M}|} = \frac{M_x}{|\vec{M}|}\vec{e}_x + \frac{M_y}{|\vec{M}|}\vec{e}_y + \frac{M_z}{|\vec{M}|}\vec{e}_z = \alpha\vec{e}_x + \beta\vec{e}_y + \gamma\vec{e}_z$$

a) Why do we have $A_{p,q,r=0}$ when at least one of the powers p,q,r is odd ?

   If we reverse the axis (π), it doesn't change the physics. We keep only terms with p, q, r even.

b) Explain why the expansion of W can be written without terms of order 2 (terms with $p+q+r=2$).

$$W^{(2)} = A_{200}\alpha^2 + A_{020}\beta^2 + A_{002}\gamma^2 = A_2\underbrace{(\alpha^2+\beta^2+\gamma^2)}_{=1} = A_2$$

c) List all possible terms of order 4. How do they group together ? Show, by considering the square of $\alpha^2+\beta^2+\gamma^2$, that these terms can be written as the sum of a constant and a sum of terms in which only squares of cosines appear.

$$\begin{aligned} W^{(4)} &= A_{220}\alpha^2\beta^2 + A_{202}\alpha^2\gamma^2 + A_{022}\beta^2\gamma^2 + A_{400}\alpha^4 + A_{040}\beta^4 + A_{004}\gamma^4 \\ &= A_{22}(\alpha^2\beta^2+\alpha^2\gamma^2+\beta^2\gamma^2) + A_4(\alpha^4+\beta^4+\gamma^4) \end{aligned}$$

$$1 + (\alpha^2+\beta^2+\gamma^2)^2 = \alpha^4+\beta^4+\gamma^4+2\alpha^2\beta^2+2\alpha^2\gamma^2+2\beta^2\gamma^2$$

Thus,

$$\alpha^4+\beta^4+\gamma^4 = 1 - 2\alpha^2\beta^2 - 2\alpha^2\gamma^2 - 2\beta^2\gamma^2$$

$$W^{(4)} = (A_{22}-2A_4)(\alpha^2\beta^2+\alpha^2\gamma^2+\beta^2\gamma^2) + A_4$$

d) Show that the expansion of W including the terms of order ≤ 6 can be written in the form

$$W(\alpha, \beta, \gamma) = K_0 + K_1(\alpha^2\beta^2 + \beta^2\gamma^2 + \gamma^2\alpha^2) + K_2\alpha^2\beta^2\gamma^2.$$

$$\begin{aligned} W^{(6)} &= A_6(\alpha^6 + \beta^6 + \gamma^6) + A_{42}(\alpha^4\beta^2 + \alpha^2\beta^4 + \alpha^4\gamma^2 + \gamma^4\alpha^2 + \beta^4\gamma^2 + \beta^2\gamma^4) + A_{222}\alpha^2\beta^2\gamma^2 \\ &= A_6(\alpha^6 + \beta^6 + \gamma^6) + A_{42}(\alpha^4(1-\alpha^2) + \beta^4(1-\beta^2) + \gamma^4(1-\gamma^2)) + A_{222}\alpha^2\beta^2\gamma^2 \\ &= (A_6 - A_{42})(\alpha^6 + \beta^6 + \gamma^6) + A_{42}(\alpha^4 + \beta^4 + \gamma^4) + A_{222}\alpha^2\beta^2\gamma^2 \end{aligned}$$

$$\begin{aligned} 1 &= (\alpha^2 + \beta^2 + \gamma^2)^3 \\ &= \alpha^6 + \beta^6 + \gamma^6 + 3\alpha^4\beta^2 + 3\alpha^2\beta^4 + 3\alpha^4\gamma^2 + 3\alpha^2\gamma^4 + 3\beta^4\gamma^2 + 3\beta^2\gamma^4 + 6\alpha^2\beta^2\gamma^2 \\ &= -2(\alpha^6 + \beta^6 + \gamma^6) + 3(\alpha^4 + \beta^4 + \gamma^4) + 6\alpha^2\beta^2\gamma^2 \end{aligned}$$

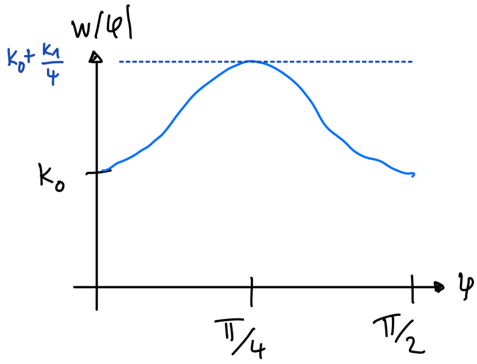
$$\begin{aligned} W^{(6)} &= \frac{1}{2}(A_{42} - A_6) + \frac{3}{2}(A_6 - A_{42})(\alpha^4 + \beta^4 + \gamma^4) + 3(A_6 - A_{42})\alpha^2\beta^2\gamma^2 + A_{42}(\alpha^4 + \beta^4 + \gamma^4) + A_{222}\alpha^2 \\ &= \frac{1}{2}(A_{42} - A_6) + \frac{1}{2}(3A_6 - A_{42})(\alpha^4 + \beta^4 + \gamma^4) + (3(A_6 - A_{42}) + A_{222})\alpha^2\beta^2\gamma^2 \\ &= \frac{1}{2}(A_{42} - A_6) + \frac{1}{2}(3A_6 - A_{42})(1 - 2\alpha^2\beta^2 - 2\beta^2\gamma^2 - 2\alpha^2\gamma^2) + (3A_6 - 3A_{42} + A_{222})\alpha^2\beta^2\gamma^2 \\ &= A_6 - (3A_6 - A_{42})(\alpha^2\beta^2 + \beta^2\gamma^2 + \alpha^2\gamma^2) + (3A_6 - 3A_{42} + A_{222})\alpha^2\beta^2\gamma^2 \end{aligned}$$

$$K_0 = A_0 + A_2 + A_4 + A_6 \qquad K_1 = A_{22} - 2A_4 - 3A_6 + A_{42} \qquad K_2 = 3A_6 - 3A_{42} + A_{222}$$

e) Consider the case when the magnetization is in the plane perpendicular to the direction [001], and at the angle φ with the direction [100]. Express the energy density $W(\varphi)$ as a function of φ and the coefficients K_0 and K_1.

$$\gamma = 0, \qquad \alpha = \cos\varphi, \qquad \beta = \cos(\pi/2 - \varphi) = \sin(\varphi)$$

$$W(\varphi) = K_0 + K_1 \cos^2\varphi \sin^2\varphi = K_0 + \frac{K_1}{4}\sin^2(2\varphi)$$



Exercise 2 : Bloch domain walls

We consider a monocrystalline ferromagnetic bar of length L, and of section A. It is assumed that the iron lattice is simple cubic, with lattice constant a. The crystalline anisotropy energy is described as in exercice 1. The ferromagnetic exchange interaction energy between two magnetic moments $\vec{\mu}_i$ and $\vec{\mu}_j$ on nearest neighbor sites is assumed to be $-J\cos\theta_{ij}$, with $J > 0$ and θ_{ij} the angle between the magnetic moments. The exchange energy between sites of larger distance is neglected.

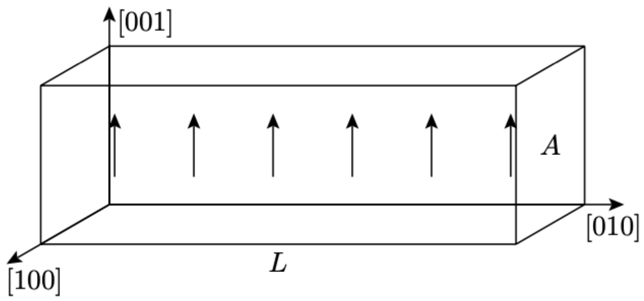
a) What is the density of atoms per unit area in a crystalline plane perpendicular to the [010] direction ? How many iron atoms are in such a section of area A ?

$$n^{\mathrm{2D}} = \frac{1}{a^2}$$

Because there is one atom in a square of a^2 area.

$$N^{\mathrm{2D}} = A \times n^{\mathrm{2D}} = \frac{A}{a^2}$$

b) Magnetized at saturation in the direction [001], the bar forms a magnetic monodomain. Calculate the crystalline anisotropy energy and the exchange energy of the single crystal, and give the total magnetic energy U_1 of the bar in the monodomain state.



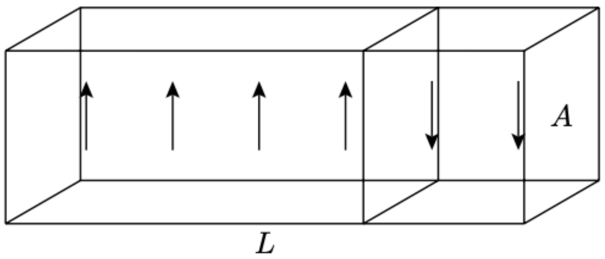
$$E_{\mathrm{ani}} = V\left(K_0 + \frac{K_1}{4}\sin^2(2\varphi)\right) \overset{\varphi=0}{=} K_0 V$$

$$n = \frac{1}{a^3} \longrightarrow \frac{LA}{a^3} = N^{\mathrm{3d}} \Longrightarrow E_{\mathrm{exchange}} = -\frac{6}{2}\frac{LA}{a^3}J = -\frac{3LA}{a^3}J$$

And thus,

$$E_{\mathrm{tot}} = K_0 V - \frac{3LA}{a^3}J$$

c) The iron bar now comprises two magnetic domains whose magnetizations are opposite and saturated. Write the magnetic energy U_2 of the bar in the form $U_2 = U_1 + \Delta U$ and give the expression of ΔU.



$$\Delta U = 2N^{\text{2D}} \times J = \frac{2JA}{a^2}$$

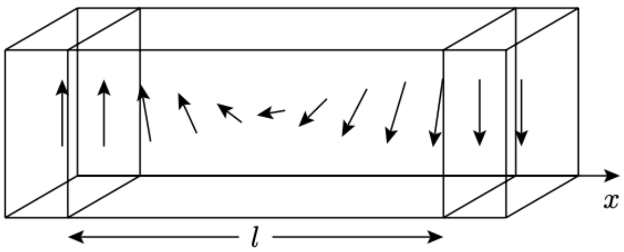
There is a 2 because we go from $-J$ to $+J$, hence a $2J$ difference.

$$U_2 = U_1 + \text{ cost of the interface}$$

$$U_2 = \left(K_0 - \frac{3}{a^3}J\right) LA + \frac{2A}{a^2}J$$

d) We now have a Bloch domain wall of thickness l between the magnetic domains of opposite saturated magnetization. In the Bloch wall, the magnetization stays in the plane perpendicular to [010], and rotates by a constant angle when moving from a crystal plane to the next one in the [010]-direction. From $x = x_0 - l/2$ to $x = x_0 + l/2$, the magnetization rotates pro- gressively by the total angle π. Show that, when $l \gg a$, the energy of the bar can be written as

$$U_{\text{DW}} = \left(K_0 - \frac{3J}{a^3}\right) AL + \left(\frac{K_1 l}{8} + \frac{\pi^2 J}{2aL}\right) A.$$



Anisotropy, let's take a slice $\mathrm{d}l$,

$$\mathrm{d}V = A\mathrm{d}l$$

$$\mathrm{d}U_{\text{ani}} = W_{\text{ani}}(\varphi)\mathrm{d}V \qquad\qquad W_{\text{ani}} = K_0 + \frac{K_1}{4}\sin^2(\varphi)$$

Thus,

$$\begin{aligned}\mathrm{d}U_{\text{ani}} &= W_{\text{ani}}(\varphi)\mathrm{d}V\\ &= W_{\text{ani}}(\varphi)A\mathrm{d}l\end{aligned}$$

And so by integration,

$$U_{\text{ani}} = \int_{-l/2}^{+l/2} \mathrm{d}lA\left(K_0 + \frac{K_1}{4}\sin^2(2\varphi)\right)$$

But,

$$\frac{\mathrm{d}l}{l} = \frac{\mathrm{d}\varphi}{\pi}$$

And so,

$$U_{\text{ani}} = \int_0^{\pi} \mathrm{d}\varphi\frac{l}{\pi}A\left(K_0 + \frac{K_1}{4}\sin^2(2\varphi)\right)$$

$$\begin{aligned}U_{\text{ani}} &= AK_0l + \frac{K_1Al}{4\pi}\int_0^{\pi}\mathrm{d}\varphi\sin^2(2\varphi)\\ &= AK_0l + \frac{K_1Al}{4\pi}\underbrace{\int_0^{\pi}\mathrm{d}\varphi\frac{1}{2}\left(1-\cos(2\varphi)\right)}_{=\pi/2}\\ &= AK_0l + \frac{K_1Al}{8}\\ &= Al\left(K_0 + \frac{K_1}{8}\right)\end{aligned}$$

If l increases, the more slices there is where the magnetic moment is not along an *easy* axis. So U_{ani} increases also, thus costing energy.

Exchange,

$$\Delta U_{\text{ex}} = -J\cos\theta_{ij} \qquad\qquad U_{\text{ex}} = -\sum_{i,j} J\cos\theta_{ij}$$

But, how many layers in a length l? l/a. For one layer to another,

$$\theta_{ij} = \frac{\pi}{\text{number of layers}}$$

Thus,

$$\theta_{ij} = \frac{\pi a}{l}$$

And so,

$$\Delta U_{\text{ex}} = \frac{Al}{a^3}\left[-J\cos\left(\frac{\pi a}{Ll}\right) + J\cos(0)\right]$$

there is $\cos(0)$ because we start with $\theta_{\text{initial}} = 0$. We have $l \gg 1$, thus

$$\cos\left(\frac{\pi a}{l}\right) \approx 1 - \frac{\pi^2 a^2}{2l^2}$$

So,

$$U_{\text{ex}} = \frac{AlJ}{a^3}\left(1 + \frac{\pi^2 a^2}{2l^2} - 1\right) = \frac{AJ\pi^2}{2al}$$

If l increases, then the energy is decreasing. The exchange prefer smoothness. Anisotropy prefers short domain wall as there are preferred axis.
So in total,

$$U_{\text{DW}} = U_{\text{ex}} + \Delta U_{\text{ani}} + U_1$$

Where we don't take the K_0 term in ΔU_{ani}.

$$U_{\text{DW}} = U_1 + A\left(\frac{J\pi^2}{2al} + \frac{K_1 l}{8}\right)$$

Be careful, just the difference with U_1 matters.

e) Determine the thickness l of the Bloch domain wall that can be expected in such a bar, and deduce the energy difference $\delta U = U_{\text{DW}} - U_1$.

We look for a minimum of U_{DW}

$$\left.\frac{\mathrm{d}U_{\text{DW}}}{\mathrm{d}l}\right|_{l=l^*} = 0 \Longleftrightarrow A\left(\frac{K_1}{8} - \frac{J\pi^2}{a(l^*)^2}\right) = 0$$

And thus,

$$l^* = \sqrt{\frac{4J\pi^2}{aK_1}} = 2\pi\sqrt{\frac{J}{ak_1}}$$

For exchange, J is big and thus we get a long wall. For anisotropy we have large K_1 and thus small wall. Coherent behavior.

f) Using the values $K_1 = 4 \times 10^4$ J.m^{-3},$J = 2 \times 10^{-21}$ J and $a = 2.9$,calculate the thickness of the wall and the energies per unit area $\Delta U/A$ and $\delta U/A$. Discuss the result.

$$l = 2\pi\sqrt{\frac{10^{-7}}{4.8}} \sim 100 \text{ mm}$$

and $a \sim 2.9$ Å. Still short compared to structure sizes.