T13. Ferromagnet model

The magnetic field in media is described by three vectors: $\vec{B}$ - magnetic field induction, $\vec{H}$ - magnetic field strength, $\vec{M}$ - magnetization (equal by definition to the magnetic moment of a unit volume of matter). There is a well-known relation between these three vectors: $\vec{B} = \mu_0(\vec{H} + \vec{M})$.

Different mechanisms can lead to magnetization, determined by the structure of the media under study. In this problem we will study the peculiarities of the magnetic structure of ferromagnetics - substances in which magnetization appears, primarily due to the reorientation of the magnetic moments of individual atoms of the crystal lattice. Examples of ferromagnets are iron, nickel, cobalt and gadolinium.

Part A. Curie-Weiss Law

Let us consider a simplified model of a crystalline ferromagnet. Let its lattice be cubic with side a and its nodes contain individual atoms. Let us introduce x, y, z axes parallel to the edges of the crystal lattice. Each atom has its own magnetic moment of constant value s, which can be directed either along or against the axis z.

A1	Find the maximum possible magnetization modulus $M_{\max}$ achievable in such a media.

The magnetic structure of a ferromagnet depends on temperature. Let us first describe its structure at sufficiently high temperatures. In this case, the substance cannot be magnetized without an external magnetic field, and the directions of magnetization of individual atoms in it are chaotic, and their statistics obeys **the Boltzmann distribution**.

Hint about the Boltzmann distribution. Consider a single atom that can be in two states 1 and 2 with different energies E_1 and E_2. Let us denote by p_1 and p_2 the probabilities of finding the atom in these states. According to the Boltzmann distribution, the formula $p_1/p_2 = \exp((E_2 - E_1)/kT)$ is true for the ratio of probabilities.

Let us study how a ferromagnet reacts to an external magnetic field in the high-temperature case. Let a sample of the substance under study at temperature T be placed in a homogeneous external magnetic field $\vec{B}$ directed along the axis z, and it is magnetized. The dependence of the magnetization $\vec{B}$ on the temperature T of the sample obeys the Curie-Weiss law:

$$\vec{M} = \vec{B}\frac{A}{T - T_C}.$$

The parameter T_C in this formula is called the Curie temperature. Next, we'll explain this law. Each atom of a ferromagnetic interacts both with the external magnetic field and with the other atoms. The latter interaction is quantum in nature and is called **exchange interaction**. The effective magnetic field $\vec{B}_{\text{eff}}$ near each atom can be represented as the sum of the external field $\vec{B}$ and the **average field** of the exchange interaction, which is proportional to the magnetization:

$$\vec{B}_{\text{eff}} = \vec{B} + b\mu_0\vec{M}.$$

Here b is a proportionality factor of order 1. Then the magnetic moment energy of the atom $\vec{s}_i$ in the effective field:

$$E_i = -(\vec{B}_{\text{eff}} \cdot \vec{s}_i) = -((\vec{B} + b\mu_0\vec{M}) \cdot \vec{s}_i).$$

Thus due to exchange interaction the magnetic moments tend to become co-directed. **However, thermal motion causes some of the spins to deviate from the general direction.**

A2	Suppose we know the value of the effective field B_{eff} in the sample under study. Find its magnetization M. Express the answer in terms of B_{eff}, a, T, s and Boltzmann constant k.

A3	Decompose the answer to the previous item into a Taylor series over B_{eff} and express the Curie temperature T_C through s, a, b, μ_0, and k.

We can see that the Curie-Weiss law predicts an unboundedly strong response of a ferromagnet to an external field near the Curie point T_C. This leads us to the idea that at this temperature the magnetic structure of the substance changes qualitatively. Indeed, it turns out that at $T < T_C$ the spins of the ferromagnetic atoms are no longer directed chaotically, but form macroscopic clusters, called **domains**, within which the spin direction is constant. In this state, the ferromagnet **can be magnetized even without an external field**.

If we heat a ferromagnet with a complex domain structure, its response to external fields will increase indefinitely as we approach the temperature T_C. Therefore, near the Curie temperature, the slightest fluctuation of the external field will destroy the domain structure of the sample and transfer it to the high-temperature phase.

Part B. Domain boundary thickness

In this part of the problem, we will estimate the thickness of the domain boundary of an anisotropic ferromagnet.

Exchange interaction energy in isotropic magnetics

Consider a sample of an isotropic ferromagnet with the cubic crystal lattice described in the previous part. Suppose now that **the magnetic moment of each atom can be directed in any direction**, not only parallel to the z-axis.

We obtain a convenient expression for the total exchange interaction energy of its atoms. It is known from quantum mechanics that the exchange interaction energy of two atoms i and j can be expressed in the following form:

$$W_{ij} = -J(|\vec{r}_i - \vec{r}_j|)(\vec{s}_i \cdot \vec{s}_j).$$

Here $J(|\vec{r}_i - \vec{r}_j|)$ is a positive rapidly decreasing function of the distance between the atoms, and $\vec{s}_i$ and $\vec{s}_j$ are the magnetic moments of the atoms. J decreases fast enough, so we can assume that **only neighboring atoms interact** (with distance between them not greater than a). Then the energy of the exchange interaction in the crystal can be written in the form:

$$W_{\text{ec}} = -\sum_{\langle i,j\rangle} J(a)(\vec{s}_i \cdot \vec{s}_j),$$

where the summation is done over all pairs of neighboring atoms in the volume of the crystal.

Suppose that the crystal is magnetized in such a way that the spin vectors of neighboring atoms differ weakly. Then we can introduce a vector function $\vec{s}(\vec{r}) = (s_x(\vec{r}), s_y(\vec{r}), s_z(\vec{r}))^T$ and use it to describe the spin directions in the lattice. Consider two atoms at points with coordinates $\vec{r}_1 = (-a/2, 0, 0)^T$ and $\vec{r}_2 = (a/2, 0, 0)^T$. Let the directions of their spins are slightly different. In the first approximation the spins of these spins are expressed as follows:

$$\vec{s}_1 \approx \vec{s}(\vec{0}) - \frac{a}{2}\frac{\partial \vec{s}}{\partial x}, \quad \vec{s}_2 \approx \vec{s}(\vec{0}) + \frac{a}{2}\frac{\partial \vec{s}}{\partial x}.$$

Their scalar product:

$$(\vec{s}_1 \cdot \vec{s}_2) = s^2 - \frac{a^2}{4}\left(\left(\frac{\partial s_x}{\partial x}\right)^2 + \left(\frac{\partial s_y}{\partial x}\right)^2 + \left(\frac{\partial s_z}{\partial x}\right)^2\right).$$

If their spins were co-directional, their contribution to the exchange energy would be minimized. However, due to non-sonadirectionality, the exchange energy increases by an amount:

$$\Delta W_{\text{ec}} = \frac{J(a)a^2}{4}\left(\left(\frac{\partial s_x}{\partial x}\right)^2 + \left(\frac{\partial s_y}{\partial x}\right)^2 + \left(\frac{\partial s_z}{\partial x}\right)^2\right).$$

If we consider the interaction of more pairs of atoms 3-4 and 5-6 with coordinates $\vec{r}_3 = (0, -a/2, 0)^T$, $\vec{r}_4 = (0, a/2, 0)^T$, $\vec{r}_5 = (0, 0, -a/2)^T$, $\vec{r}_6 = (0, 0, a/2)^T$, then we obtain that the volume density of the exchange energy w at point $(0, 0, 0)$ is proportional:

$$w(\vec{0}) \sim \left((\nabla s_x)^2 + (\nabla s_y)^2 + (\nabla s_z)^2\right)\Bigg|_{\vec{r}=\vec{0}}, \quad \nabla s_i(\vec{r}) = \left(\frac{\partial s_i}{\partial x}, \frac{\partial s_i}{\partial y}, \frac{\partial s_i}{\partial z}\right)^T.$$

It turns out that the energy of the exchange interaction can be rewritten as an integral over the volume of the ferromagnetic V, which is convenient for analysis:

$$W_{\text{ec}} = \alpha \int_V \left((\nabla s_x)^2 + (\nabla s_y)^2 + (\nabla s_z)^2\right)\mathrm{d}V.$$

Here $\alpha > 0$ is some proportionality factor that can be estimated from thermodynamic considerations.

B1	Estimate the value of α. Express the answer in terms of a, k, T_C, and s.

Energy of an anisotropic ferromagnet

Let the sample under study be mechanically compressed along the z-axis. Then it ceases to be magnetically isotropic. The z-axis will become a dedicated direction of anisotropy and all spins of the lattice will tend to orient parallel to it. The effect of anisotropy on the energy of the sample can be taken into account by introducing the bulk density associated with anisotropy:

$$W_{\text{ob}} = \int_V \left[\alpha\left((\nabla s_x)^2 + (\nabla s_y)^2 + (\nabla s_z)^2\right) - \beta s_z^2\right]\mathrm{d}V, \quad \beta > 0.$$

We will consider the anisotropy weak, so $\beta \ll \alpha a^2$.

Calculation of the thickness of the domain boundary

Let us proceed to the calculation of the domain boundary thickness. Let the sample have an anisotropy axis z, all elementary magnetic moments in it are oriented perpendicular to the axis x ($s_x \equiv 0$) and in each plane of the form $x = \text{const.}$ all spins are directed equally (i.e., $\vec{s}$ depends only on x). We can introduce an angle $\theta(x)$ between the magnetic moment and the z-axis, then $\vec{s}(x)$ is expressed as follows:

$$s_x(x) = 0, \quad s_y(x) = s\sin\theta(x), \quad s_z(x) = s\cos\theta(x).$$

B2	Write the expression for the total energy of exchange interaction in a rectangular parallelepiped with sides $L \times D \times D$ ($\lvert x\rvert \le L/2, \lvert y\rvert \le D/2, \lvert z\rvert \le D/2$) as an integral of the form $$W_{\text{ec}} = \int_{-L/2}^{L/2} F(x, \theta(x))\mathrm{d}x.$$

If for a function $\theta(x)$ the energy found in the previous paragraph is minimal, then $\theta(x)$ satisfies the Euler-Lagrange equation:

$$\frac{\partial F}{\partial \theta} = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial \theta'}, \qquad \theta' \equiv \frac{\mathrm{d}\theta}{\mathrm{d}x}$$

B3	Express $\theta'' \equiv \mathrm{d}^2\theta/\mathrm{d}x^2$ through α, β, and θ.

Let the plane $x = 0$ be the center of the boundary between two domains. The first domain is located in the region $x < 0$ and in it almost all spins are oriented against the axis z, and the second domain is located in the region $x > 0$ and in it spins are oriented along the axis z.

B4	Write the boundary conditions for solving the equation obtained in the previous paragraph. Specifically, find $\theta(x = 0)$, $\theta(x \to \infty)$, $\theta(x \to -\infty)$, $\theta'(x \to \infty)$, $\theta'(x \to -\infty)$.

B5	Find the expression for $\theta(x)$ in terms of x, α, and β.

B6	Express the thickness of the boundary between the domains Δ through α and β and show that $\Delta \gg a$.