Thermal Conductivity of Magnets in a Wide Range of Temperatures

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Abstract
The thermal conductivity coefficient of a ferromagnet $\kappa$ is estimated at temperatures lying near the phase transition point, that is, with $\varepsilon \ll T_c$, $T = T_c - \varepsilon$, where $\varepsilon$. The calculations are based on the method of the quasi-classical kinetic equation, and it is shown that $\kappa = \kappa_0 \left(1 - \frac{T}{T_c} + \delta_0\right)^{\frac{5}{2}}$ with the critical index equal to $\frac{5}{2}$, and $\delta_0 = \frac{H_a}{H_E}$, where $H_a$ is the magnetic anisotropy field, $H_E$ is the exchange field.

Keywords: magnetic phase transition temperature, quasi-classical kinetic equation, thermal conductivity coefficient.

1. Introduction
Upon careful acquaintance with a large number of literature sources describing the physical properties of magnetic substances at temperatures of the magnetic phase transition range (for example, see [1] – [10]), despite the almost century-old history of this issue, we did not find an analytical calculation of the temperature dependence of the thermal conductivity coefficient of ferromagnets $\kappa(T)$ with $T = T_c \pm \varepsilon$, where $T_c$ is the Curie temperature, and $\varepsilon \ll T_c$.

And although the general theory of phase transitions, both macroscopic [11] – [13] and microscopic [14] - [18], has long been built up, and the authors have deservedly received Nobel Prizes, some issues for some reason still remained ignored and were not covered in the literature. That is why the purpose of this report is to close this small gap associated with the calculation of the critical index of the thermal conductivity coefficient in the region of the magnetic phase transition temperature. Experimental measurements devoted to this issue [19] – [21] (which is typical of any other physical characteristics in the field $T = T_c$) indicate a strong increase in thermal conductivity near $T_c$, the value of which $\kappa_{\text{max}} = \kappa(T_c)$ can be calculated analytically, and which, as we will see, has a finite value.

Looking ahead, let us note that the value of this maximum is determined by the value

$$\kappa_{\text{max}} = \kappa_0 \left(\frac{H_E}{H_a}\right)^{\frac{3}{2}},$$

where $\kappa_0$ is a representative coefficient of thermal conductivity, $H_a$ is the magnetic anisotropy field, $H_E$ is the exchange magnetic field, $J_{\text{ex}}$ is the energy of the exchange interaction, and $\mu_e$ is the Bohr magneton.

2. The interaction Hamiltonian with $T < T_c$
In the theory of phase transitions, concerning the non-equilibrium properties of matter, the necessary condition is always the knowledge of the corresponding relaxation time.

Specifically, when it comes to thermal conductivity, in order to calculate $\kappa$, it is necessary to have an idea of the relaxation time, which, in the case of a ferromagnet, is resulting from the interaction between the magnon and phonon subsystems.

Since we are talking about the gas-kinetic approximation, the basic calculation formula in the isotropic case should be, according to the general rules for its calculating [22] – [24], as follows:

$$\kappa = \frac{1}{3(2\pi)^3} \int v^2 \tau_{\mu-\rho} (k) d^3k,$$  (1)
where \( v = \frac{1}{h} \frac{\partial \varepsilon_k}{\partial k} \) – is the group velocity of magnons, 
\[
\varepsilon_{ex} = J_{ex} (ak)^2 + bk_n T_c \left( 1 - \frac{T}{T_c} \right) + \mu_e H_a = \text{their}
\]
dispersion, \( J_{ex} \) is an exchange integral, \( T_c \) is Curie temperature, \( \alpha - \) is interatomic distance, \( b - \) is dimensionless constant, \( \mu_e \) is Bohr magneton, 
\( H_a \) is magnetic anisotropy field, \( h \) is Planck constant, \( k - \) is magnon wave vector, \( k_B \) is Boltzmann constant, \( \tau_{m-\text{ph}} (k) \) is magnon-phonon relaxation time.

Hereinafter, we will use the energy system of units, in which we assume that the Boltzmann constant is \( k_B = 1 \), and for convenience, we will also assume that the Planck constant is \( h = 1 \). This will not lead to confusion in dimensions (see below).

Since the group velocity of magnon is \( v = 2J_{ex}a^2k \), then in the isotropic case we can always assume that \( a^2k = 4\pi k^2 \), and therefore, from (1) we have
\[
\kappa = \frac{2J_{ex}a^2}{3\pi^2} \int_{k_0}^\pi \frac{1}{k^3} \tau_{m-\text{ph}} (k) dk ,
\]
where the lower limit of integration can be determined only after analyzing the theory of conservation of energy and momentum for a particular magnon-phonon type of interaction (see inequality (21)).

To this end, we need to introduce the magnon – phonon interaction energy, which is easy to write down for the isotropic case, considering the crystal symmetry to be cubic.

We can represent the corresponding interaction in a single form, as
\[
H_{m-\text{ph}} = \gamma \int_V M M_k u_{ik} dV .
\]
where \( \gamma - \) is the dimensionless striction constant of the order of unity, \( M = (M_i) - \) is the order parameter, i.e., the magnetic moment per unit volume of the ferromagnet, \( u_{ik} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right) \) – is the strain tensor, \( u_i = (u_i) - \) is the strain vector, \( V - \) is the volume of the body.

By the way, it is worth noting that there can be no interaction of \( H_{\text{int}} = \gamma \int_V M M_k u_{ik} u_{in} dV \) type in crystals with any spatial symmetry. This is simply due to the physical fact that any type of interaction must satisfy the rule of invariance with respect to the time inversion operation, i.e., \( H_{\text{int}} (t) = H_{\text{int}} (-t) \) where \( t - \) is time. Since the magnetization vector is an axial vector with respect to replacement \( t \rightarrow -t \), that is \( M (-t) = -M (t) \), this indicates the impossibility of this type of interaction; although it should be noted that the theorem of conservation of energy and momentum do not prohibit this type of interaction at all.

To rewrite the interaction (3) in the language of the operators of creation and annihilation of magnons and phonons, it must be represented in a second – quantized form. To do this, it should be remembered that in accordance with the Holstein-Primakov transformations [25], we have the right to write down that
\[
\begin{align*}
M^+ &= M_y + i M_y \approx M_0 \sqrt{2S} a (r), \\
M^- &= M_y - i M_y \approx M_0 \sqrt{2S} a^+ (r),
\end{align*}
\]
where \( M_0 = \frac{\mu_e}{a^3} \sqrt{1 - \frac{T}{T_c}} + \delta_0 \) – is the spontaneous magnetization in the region of the Curie temperature, \( S - \) is the spin of the atom, \( a^+ (a) - \) is the magnon creation (annihilation) operator at a local point with a radius vector \( r \). The expression for the non-dimensional value \( \delta_0 \) is given below.

In \( k - \) representation, the magnon creation and annihilation operators can be represented as a Fourier series
\[
\begin{align*}
a (r) &= \frac{1}{\sqrt{N}} \sum_k a_k e^{ikr}, \\
a^+ (r) &= \frac{1}{\sqrt{N}} \sum_k a^*_k e^{-ikr},
\end{align*}
\]
where \( N - \) is the total number of atoms in the ferromagnetic material.

Quantization of the strain vector is also easily accomplished by using a simple Fourier decomposition
\[
u = \sum_{q,\alpha} e_{\alpha} \sqrt{\frac{\hbar}{\rho \omega_{\alpha} (q)V}} \left( b_{\alpha}^* (q) + b_{-\alpha} (q) \right) e^{iqr} .
\]
According to (6), the components of the strain tensor can then be represented as
\[ \varepsilon_{ik} = \frac{i}{2} \sum_{q,a} (e_{ia} q_i + e_{ai} q_a) \sqrt{\frac{h}{\rho \omega_k(q)}} (b_{q}^{*} + b_{-q}^{*}) e^{i\phi} \] (7)

After applying (5) and (7) to definition (3) as a result of simple transformations taking into account the rule
\[ \int_V e^{i(k_i - k_i^\prime - q_i)} dV = V \Delta (k_i - k_i^\prime \pm q_i), \] (8)

we get the desired interaction
\[ H_{m-pb} = \sum_{k_i,k_i^\prime} \Psi(k_i,k_i^\prime,q,q,a) a_i^{*} a_i (b_{q}^{*} + b_{q}^{*}) \Delta(k_i - k_i^\prime + q_i) + c.c. \] (9)

where abbreviation c.c. means a complex-conjugate quantity, and indices 1, 2 of the creation and annihilation operators mean reduction 1 \( \equiv k_1 \), 2 \( \equiv k_2 \), and the interaction amplitude is defined as
\[ \Psi(k_i,k_i^\prime,q,q,a) = i \frac{4 \pi \rho M V}{N \sqrt{V}} \sqrt{\frac{h}{\rho \omega_{k_i^\prime}(q)}} (e_{ia} q_i - e_{ai} q_a). \] (10)

It is quite obvious that in the absence of interaction, the main Hamiltonian can be written as
\[ H_0 = \frac{1}{N} \sum_k \varepsilon_k a_i^{*} a_i + \frac{1}{N} \sum_q \omega_q(q) b_{q}^{*} b_{q}. \]

where \( \varepsilon_k \) and \( \omega_q(q) \) are defined above.

3. Calculation of the relaxation time in the region of the phase transition temperature

If we use a quasi-classical kinetic equation (see, for example, [26] – [29]), namely, the equation
\[ \frac{\partial n_k}{\partial t} = L \{ n_k, \bar{f}_q \}, \] (11)

where \( L \) is the collision integral, \( n_k \) is the magnon distribution function, \( \bar{f}_q \) is the equilibrium distribution function of phonons, which are considered a thermostat and, at high temperatures in the region of the Curie temperature, it can be represented as a decomposition of the Bose distribution
\[ \bar{f}_q = \frac{1}{e^{\varepsilon_k / T} - 1} \approx \frac{T_c}{\varepsilon_k}. \] (12)

Before proceeding to specific calculations, it is worth noting that equation (11) will be correct, if condition
\[ \varepsilon_k \geq \frac{h}{\tau_{m-pb}(k)}, \] where \( \tau_{m-pb}(k) \) – magnon is the phonon relaxation time, is satisfied. As we will see later (see Formula (20)), this condition is satisfied near the phase transition point, and it is quite possible to use equation (11).

According to interaction (9), the collision integral will be
\[ L[n_k] = 2 \pi \sum_{k_i^\prime} \Psi(k_i^\prime,k_i,q,q,a) n_{k_i^\prime^\prime} a_i^{*} a_i (b_{q}^{*} + b_{q}^{*}) \Delta(k_i^\prime - k_i + q_i) + c.c. \] (13)

+ \[ 2 \pi \sum_{k_i^\prime} \Psi(k_i^\prime,k_i^\prime,q,q,a) n_{k_i^\prime^\prime} a_i^{*} a_i (b_{q}^{*} + b_{q}^{*}) \Delta(k_i^\prime^\prime - k_i^\prime + q_i) \delta(\varepsilon_k - \varepsilon_{k_i^\prime^\prime} + \varepsilon_{k_i^\prime}). \] (14)

where the presence of the delta function automatically takes into account the law of energy conservation.

According to (15), the relaxation time in the "tau approximation" will be
\[ \tau_{k_i^\prime} = \frac{1}{e^{T_c / T} - 1} \approx \frac{T_c}{\varepsilon_k}. \] (15)

As a result, instead of (14), we get
\[ \tau_{k_i^\prime} = \frac{1}{e^{T_c / T} - 1} \approx \frac{T_c}{\varepsilon_k}. \] (16)

After summing by \( k_i \), from (16) we have
\[ \sum q(\ldots) = \frac{V}{2\pi} \int (\ldots) d^3 q \] (18)

allows us to get the following intermediate expression
\[ \frac{1}{e^{T_c / T} - 1} \approx \frac{q_{i1} + q_{i2}}{2}, \] (19)

with the parameters
\[ F = \frac{T_c \varepsilon_k^2}{3 \pi \rho} \rho M V, \] (20)

\[ G = \frac{T_c \varepsilon_k^2}{6 \pi \rho} \rho M V, \]

\[ \beta = a^2 \omega_k, \]

\[ q_{i1} = \frac{c}{\beta} + 2k, \quad q_{i2} = \frac{c}{\beta} + 2k, \]

In fact, simple but rather cumbersome calculations of the integrals appearing in (19) lead to the following final result for the relaxation time of interest.
\[
\frac{1}{\epsilon_{\alpha\beta}(k)} = \frac{F}{2c^2} \left( 1 - \frac{c^2}{4\beta^2 k^2} \right) e^{\frac{c^2}{4\beta^2 k^2}} \ln \left[ \frac{e^{\frac{c^2}{4\beta^2 k^2}} - e_{\alpha\beta}}{e^{\frac{c^2}{4\beta^2 k^2}} - e_{\beta\alpha}} \right] + \frac{F e_0}{4\beta h k c^2} \ln \left[ \frac{e_{\alpha\beta} + c_{\alpha\beta}(q)}{e_{\alpha\beta} - c_{\alpha\beta}(q)} \right] + \frac{AGk}{3} \left( k^2 + \frac{\omega_0}{\beta} \right)^2 - \left( k^2 - \frac{\omega_0}{\beta} \right)^2 \right],
\]

(21)

where \( q_{1,2} \) are defined in (20), and the magnon wave vector must be "clamped" in the segment

\[
\sqrt{\frac{\omega_0}{\beta}} = k_0 \leq k \leq \frac{\pi}{a}.
\]

(22)

Analysis of expression (21) shows that only large magnon wave vector values will make the greatest contribution to the thermal conductivity coefficient. This means that the last term in (21) will be the most significant. Leaving only it and applying the result to the general determination (2), we get

\[
\kappa \approx \frac{\rho a^3 \omega_0^2 h c^2}{4 \gamma S a^3 M_0^2} \frac{\pi}{\beta^2} \left( \frac{\pi}{\beta} \right) \frac{d k}{(ak)^2} + b \left( 1 - \frac{T}{T_c} \right) + \frac{H_a}{H_E}.
\]

(23)

Due to the convergence of this integral, we can put the lower limit of integration equal to zero, and the upper limit equal to infinity.

If we assume that at point \( T = T_c \), for an extremely short period of time \( \tau \), which is significantly less than all the relaxation times, the magnetic order instantly appears, then we have the right to write the following expression for the thermal conductivity coefficient

\[
\kappa \approx \frac{\kappa_0}{\left( 1 - \frac{T}{T_c} + \delta_0 \right)^2} \left( b \left( 1 - \frac{T}{T_c} \right) + \frac{H_a}{H_E} \right).
\]

(24)

where

\[
\kappa_0 \approx \frac{\pi \rho a^2 \omega_0^4 \alpha^2}{4 \gamma S \mu^2}.
\]

(25)

Formulas (24), (25) give an answer to the question posed at the beginning of the article, and the dimensionless parameter \( \delta_0 \) that appears in the determination \( M_0 \) (see formulas (4)) according to (24) is

\[
\delta_0 = \frac{H_a}{H_E}.
\]

That is, it should be as follows

\[
M_0 = \frac{\mu_c}{\alpha^2} \sqrt{1 - \frac{T}{T_c}} + \frac{H_a}{H_E}.
\]

(26)

It would seem that with \( T = T_c \) we have a small but finite value of the order parameter. However, it should be understood that we are talking about temperatures just below the phase transition point, that is, we should assume that \( T = T_c - \epsilon \), and the magnetic anisotropy field behaves as

\[
H_a = \begin{cases} 0, & \text{if } T \geq T_c, \\ H_a, & \text{if } T < T_c. \end{cases}
\]

(27)

That is, near the Curie point, the energy of magnetic anisotropy begins to form and the thermal conductivity should increase sharply, which is in accordance with the general principles of the theory of phase transitions. Its maximum value can be estimated as

\[
\kappa_{\text{max}} \approx \kappa_0 \left( \frac{H_E}{H_a} \right)^2.
\]

(28)

4. The thermal conductivity of a paramagnet with \( T > T_c \)

It is quite clear that in this temperature range, which is not very far from the melting point, the magnetic moment in the absence of an external magnetic field is zero, and, therefore, there should be no magnetic interactions, as well as there should be no energy of magnetic anisotropy. This means that heat transfer in the paramagnetic phase can only occur due to acoustic phonons, even if there is no crystal order. This is obviously due to the fact that there is always an inhomogeneous density of material \( \rho(\mathbf{r}) \), which, under the theory of elastic deformation, can be represented as a ratio \( \rho = \rho_0 \left( 1 + \text{div}\mathbf{u} \right) \), where \( \rho_0 \) is the unperturbed density of the material.

This means that to calculate the unique phonon – phonon relaxation time in this case, we can proceed from an isotropic Hamiltonian of the form (see [27])

\[
H_{\text{ph}} = \frac{\theta}{V} \int u_\alpha u_\beta u_\gamma dV,
\]

(29)

where \( \theta \) is some characteristic energy corresponding, in the order of magnitude, to the Debye energy \( \theta_D \).

By applying (7) here, taking into account (8), we find

\[
H_{\text{ph}} = \sum_{\{\alpha\}} \psi \left( \{q, \alpha\} \right) b_\alpha^+ b_\beta \Delta \left( q_0 - q_\alpha + q_\beta \right) + c.c.
\]

(30)

where we have introduced the abbreviations

\[
\{q, \alpha\} = \{q_1, \alpha_1; q_2, \alpha_2; q_3, \alpha_3\}
\]

\[
b_\alpha^+ (b_\alpha) \equiv b_\alpha (b_\alpha^+).
\]

The interaction amplitude is

\[
\psi = \frac{\theta^N}{\sqrt{\delta_0(q) \delta_0(q') \delta_0(|q - q'|)}} \left( k^2 \right) \left( c_{\alpha_1 \beta_1} + c_{\alpha_2 \beta_2} + c_{\alpha_3 \beta_3} \right) \left( c_{\beta_1 \alpha_1} + c_{\beta_2 \alpha_2} + c_{\beta_3 \alpha_3} \right).
\]

(31)

In this case, the main Hamiltonian will be
According to (30), the collision integral will be

\[ L = 2\pi \sum_{q_1, q_2, \ldots, q_n} \left| f \right|^2 \left( (1 + f) f - f (1 + f) f \right) (q_1, q_2, \ldots, q_n) \delta (q_1, q_2, \ldots, q_n, q_1, q_2, \ldots, q_n) + \]

\[ + 2\pi \sum_{q_1, q_2, \ldots, q_n} \left| f \right|^2 \left( (1 + f) f - f (1 + f) f \right) (q_1, q_2, \ldots, q_n) \delta (q_1, q_2, \ldots, q_n, q_1, q_2, \ldots, q_n). \]

And so, the relaxation time we are interested in will be

\[ \tau_{ph}(q) = \frac{2\pi}{q} \sum_{q_1, q_2, \ldots, q_n} \left| f \right|^2 \left( (1 + f) f - f (1 + f) f \right) (q_1, q_2, \ldots, q_n) \delta (q_1, q_2, \ldots, q_n, q_1, q_2, \ldots, q_n) + \]

\[ + 2\pi \sum_{q_1, q_2, \ldots, q_n} \left| f \right|^2 \left( (1 + f) f - f (1 + f) f \right) (q_1, q_2, \ldots, q_n) \delta (q_1, q_2, \ldots, q_n, q_1, q_2, \ldots, q_n). \]

As

\[ \tau = \frac{T}{\omega(q)}, \]

then from (33) we have

\[ \frac{1}{\tau_{ph}(q)} = 2\pi T \sum_{q_1, q_2, \ldots, q_n} \left| f \right|^2 \left( \frac{1}{\omega_1} - \frac{1}{\omega_2} \right) \Delta(q_1 - q_2, q_1, q_2) \delta (\omega_1 - \omega_1, \omega_2) + \]

\[ + 2\pi \sum_{q_1, q_2, \ldots, q_n} \left| f \right|^2 \left( \frac{1}{\omega_1} + \frac{1}{\omega_2} \right) \Delta(q_1 - q_2, q_1, q_2) \delta (\omega_1 - \omega_1, \omega_2). \]

where \( \omega = \omega(q) \).

Taking into account the conservation theory and after transition from summation to integration according to rule (18), taking into account the explicit expression for the interaction amplitude (31), and taking into account the properties of the delta function, we obtain, as a result of integration,

\[ \frac{1}{\tau_{ph}(q)} = \frac{2T}{8\pi} \frac{\Omega^3 V}{N c_s^2} \left( \frac{N}{\rho c_s V} \right)^3 q \left( q^3 + q_0^3 - 1,5qq_0^2 \right) \]

(34)

where \( q_0 = \frac{\pi}{V} \left( \frac{N}{1} \right)^{1/3} \).

By applying (34) to the general expression for the thermal conductivity coefficient

\[ \kappa_{ph} = \frac{c_v^2}{6\pi} \int_0^q q^2 \tau_{ph}(q) dq, \]

we will have

\[ \kappa_{ph}(T) = \frac{27}{4\pi^2} \frac{\rho \lambda c_v^2}{T^2 \theta^2} \left( \frac{V}{N} \right)^{7/3}. \]

(35)

For a numerical estimate \( \kappa, \) we can assume that

\[ \frac{V}{N} \approx \bar{a}^3, \]

where \( \bar{a} \) is some average interatomic distance. By applying specific numerical values

\[ \rho = 10^4 \text{ cm}^{-3}, \ c_v = 10^4 \text{ cm}^2 \text{ s}^{-1}, \ \pi = 10^{-4} \text{ cm}, \ T = 10^7 \text{ K}, \ E = 10^{-17} \text{ erg}, \ \theta \approx 10^7 \text{ K}, \ 10^{-14} \text{ erg} \]

to (35), from here we get \( \kappa_{ph} \approx 10^{23} \frac{1}{\text{cm} \cdot \text{s}}. \) If we put

\[ T = T_c \]

to (35) and compare it with (28), we see that

\[ \kappa_{max} > \kappa_{ph}(T_c). \]

Therefore, the jump in thermal conductivity during transition from the paramagnetic to the magnetic phase will be the value of

\[ \Delta = \kappa_{max} - \kappa_{ph}(T_c). \]

The ratios (36), (37) allow us to construct the dependence \( \kappa(T) \) in a wide range of temperatures up to the melting point, which is shown in Figure 1.

5. Conclusion

In conclusion, we should once again pay attention to some of the results obtained above.

1. The thermal conductivity coefficient of a ferromagnet in the vicinity of the phase transition temperature is calculated using a quasi-classical kinetic equation;

2. A critical power-law growth index is found and it is shown that \( \kappa = \kappa_0 \left( \frac{T}{T_c} \right)^{-\lambda} \), where

\[ \lambda = \frac{5}{2} \] (see formula (24)).

3. The phonon thermal conductivity in the paramagnetic phase with \( T > T_c \) has been compared with the thermal conductivity in the magnetic phase with \( T \leq T_c \), and the jump in the thermal conductivity at point \( T = T_c \) has been calculated.

4. A graphical interpretation of the obtained result is given in a wide temperature range.

References


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