LANDAU EFFECTIVE HAMILTONIAN AND ITS APPLICATION TO MAGNETIC SYSTEMS

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The Landau definition of the effective Hamiltonian (of the nonequilibrium free energy) is realized in a microscopic theory. According to Landau remark, the consideration is based on classical statistical mechanics. In his approach nonequilibrium states coinciding with equilibrium fluctuations are taken into account (the Onsager principle). The definition leads to the exact fulfillment of the Boltzmann principle written in the form with the complete free energy. The considered system is assumed to consist of two subsystems. The first subsystem is an equilibrium one. The second subsystem is a nonequilibrium one and its state is described by quantities that are considered as order parameters. The effective Hamiltonian is calculated near equilibrium in the form of a series in powers of deviations of the order parameters from their equilibrium values. The coefficients of the series are expressed through equilibrium correlation functions of the order parameters. In the final approximation correlations of six and more order parameters are neglected and correlations of four parameters are assumed to be small that leads to the corresponding perturbation theory. The developed theory is compared with the phenomenological Landau theory of phase transitions of the second kind. The obtained results are concretized for paramagnetic-ferromagnetic system. The consideration is restricted by paramagnetic phase.

Keywords: effective Hamiltonian, the Boltzmann principle, the Onsager principle, phase transitions of the second kind, correlation functions of the order parameter, small correlation function approximation.

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1. Introduction

Following Landau [1] modern theory of phase transitions of the second kind is based on an expression for the thermodynamic potential of a nonequilibrium state described by equilibrium variables which are natural for this potential and some addition of variables η_a named order parameters. The considered system is assumed to consist of two subsystems. The first subsystem is an equilibrium one with the temperature T . The second subsystem is a nonequilibrium one and its state is described by the order parameters. In the vicinity of the phase transition temperature T_c parameters η_a are considered to be small and, for example, the Landau free energy has the form of a truncated expansion in series of η_a powers

$$F(T,n,\eta) = F_0(T,p) + \sum_{a_1} \alpha_{a_1}(T,n)\eta_{a_1} + \sum_{a_1,a_2} A_{a_1a_2}(T,n)\eta_{a_1}\eta_{a_2} + \\ + \sum_{a_1,a_2,a_3} C_{a_1a_2a_3}(T,n)\eta_{a_1}\eta_{a_2}\eta_{a_3} + \sum_{a_1,a_2,a_3,a_4} B_{a_1a_2a_3a_4}(T,n)\eta_{a_1}\eta_{a_2}\eta_{a_3}\eta_{a_4} \,. \quad (1)$$

The proposed by Landau theory considers functions of T,n in this expression as unknown ones, but their general properties were discussed in details by him. However, Landau did not propose a microscopic theory for calculating these functions. Nevertheless, he systematically considered [1-3] potential $F(T,n,\eta)$ as result of the Legendre transformation of the equilibrium free energy $F(T,n,h)$ in the presence of external field h_a of the form $\hat{U} = \sum_a h_a \hat{\eta}_a$ (hereafter cap over a quantity g denotes its microscopic value $\hat{g}$; in the considered here case of a system described by classical mechanics $\hat{g}$ is a function of the phase variables). A little bit later this idea was independent by elaborated in details by Leontovich [4, 5]. This approach (the Landau-Leontovich definition) gives the function $F_{LL}(T,n,\eta)$ which was systematically investigated in our paper [6] where its realization is constructed in a microscopic theory.

First of all, the modern theory of phase transitions of the second kind is a phenomenological one. It is assumed that basic properties of phase transitions do not depend on concrete expressions for coefficient functions in the expansion (1) [7]. However some investigations are devoted to development of a microscopic theory and calculation of nonequilibrium free energy especially. See for example a substantial review [8] of microscopic theory in the vicinity of the critical point of a liquid–vapor system.

In the present paper a general idea of nonequilibrium free energy construction that belongs to Landau too is realized in a microscopic theory. This approach starts from the Boltzmann formula for distribution $w(\eta)$ of order parameter η_a in an equilibrium system that is written in the form

$$w(\eta) = e^{\frac{F(T,n)-F_L(T,n,\eta)}{T}}, \qquad \int d\eta w(\eta) \equiv 1 \qquad (d\eta \equiv \prod\nolimits_a d\eta_a) \tag{2}$$

where $F(T,n)$ is exact equilibrium free energy of the system (the temperature T is measured in energy units). According to Pitaevskii [1], Landau considered this formula as a definition of nonequilibrium free $F_L(T,n,\eta)$ and proposed to name it as the effective Hamiltonian of the system in the space of order parameters η_a (see about terminology also [9]). Formula (2) is the analog of the canonical Gibbs distribution

$$w = e^{\frac{F(T,n)-\hat{H}}{T}}, \quad \mathrm{Sp}\, w \equiv 1 \tag{3}$$

where $\hat{H}$ is the Hamiltonian of the system. Hereafter the notation

$$\overline{g} = \mathrm{Sp}\, w \hat{g} \tag{4}$$

for average equilibrium value $\overline{g}$ of a quantity g is used (to be short Sp denotes integration over phase space).

Note, that the Boltzmann formula is not exact one for the Landau–Leontovich definition of the nonequilibrium free energy $F(T,n,\eta)$ (see discussion in [4, 5]). Exact microscopic expression for distribution function $w(\eta)$ is given by standard expression

$$w(\eta) = \mathrm{Sp}\, w \delta(\eta - \hat{\eta}) \qquad (\delta(\eta - \hat{\eta}) \equiv \prod\nolimits_a \delta(\eta_a - \hat{\eta}_a)). \tag{5}$$

Thus, the definition (2), (5) accounts only nonequilibrium states that arise in equilibrium fluctuation. This restriction can be named the Onsager principle that was introduced by him in his theory of the kinetic coefficients symmetry.

Finally the Landau effective Hamiltonian is given by the formula

$$F_L(\eta) = -T \ln \mathrm{Sp}\, e^{-\frac{\hat{H}}{T}} \delta(\eta - \hat{\eta}) \tag{6}$$

(hereafter variables T, n are omitted from the notation $F(T,n)$, $F_L(T,n,\eta)$). This formula coincides with the Landau expression given in [2] without discussion.

The present paper is constructed as follows. The section 2 develops general theory for calculation of the Landau effective Hamiltonian in a perturbation theory in small order parameters. The section 3 is devoted to an application of the elaborated general theory to paramagnetic–ferromagnetic phase transition.

2. The Landau effective Hamiltonian

Let us turn to the calculation of the Landau free energy (the Landau effective Hamiltonian) $F_L(\eta)$ that consequently gives

$$e^{-\frac{F_L(\eta)}{T}} = \mathrm{Sp}\, e^{-\frac{\hat{H}}{T}} \delta(\eta - \hat{\eta}) = T^s\, \mathrm{Sp}\, e^{-\frac{\hat{H}}{T}} \delta\big((\eta - \hat{\eta})/T\big) = \\ = \left(\frac{T}{2\pi}\right)^s \int du\, \mathrm{Sp}\, e^{-\frac{\hat{H}}{T}} e^{\frac{i\sum_a u_a(\eta_a - \hat{\eta}_a)}{T}} \tag{7}$$

with account for the notations and formulas used

$$du = \prod_a du_a\,, \quad \int du = \prod_a \int_{-\infty}^{\infty} du_a\,, \qquad \delta(\eta_a) = \frac{1}{2\pi}\int_{-\infty}^{\infty} du_a e^{i u_a \eta_a}\,. \tag{8}$$

The equilibrium function of Gibbs distribution in the presence of external field $\hat{U} = \sum_a h_a \hat{\eta}_a$ has a form

$$w_h = e^{\frac{F_h - [\hat{H} + \sum_a h_a \hat{\eta}_a]}{T}}\,, \ \mathrm{Sp}\, w_h = 1\,. \tag{9}$$

Here F_h is the free energy of the system in the presence of an external field, which we use in calculations as an auxiliary value. Function F_h is given by the formula

$$e^{-\frac{F_h}{T}} = \mathrm{Sp}\, e^{-\frac{\hat{H} + \sum_a h_a \hat{\eta}_a}{T}}\,, \tag{10}$$

which allows us to rewrite the expression (7) for Landau free energy in the form

$$e^{-\frac{F_L(\eta)}{T}} = \left(\frac{T}{2\pi}\right)^s \int du\, \mathrm{Sp}\, e^{-\frac{\hat{H} + i\sum_a u_a \hat{\eta}_a}{T}} e^{\frac{\sum_a i u_a \eta_a}{T}} = \left(\frac{T}{2\pi}\right)^s \int du\, e^{\frac{\sum_a i u_a \eta_a}{T}} e^{-\frac{F(iu)}{T}}\,. \tag{11}$$

Let us introduce now generating function $\mathbf{F}(u)$ for equilibrium averages

$$\overline{\hat{\eta}_{a_1} \ldots \hat{\eta}_{a_n}} \equiv \mathrm{Sp}\, w \hat{\eta}_{a_1} \ldots \hat{\eta}_{a_n} \tag{12}$$

in the absence of an external field by the formula

$$\mathbf{F}(u) = \mathrm{Sp}\, w e^{-\frac{\sum_a u_a \eta_a}{T}}\,. \tag{13}$$

Obviously, standard identities are true for it

$$\mathbf{F}(u) = \sum_{n=0}^{\infty} \frac{(-1)^n}{T^n n!} \sum_{a_1 \ldots a_n} u_{a_1} \ldots u_{a_n} \overline{\hat{\eta}_{a_1} \ldots \hat{\eta}_{a_n}}\,, \qquad \left.\frac{\partial^s \mathbf{F}(u)}{\partial u_{a_1} \ldots \partial u_{a_s}}\right|_{u=0} = \frac{(-1)^n}{T^n} \overline{\hat{\eta}_{a_1} \ldots \hat{\eta}_{a_s}} \tag{14}$$

According to (10), the definition (13) of the generating function $\mathbf{F}(u)$ gives the following formula for the free energy of the system in the external field

$$e^{\frac{F-F_h}{T}} = \mathbf{F}(h). \tag{15}$$

With taking this into account, the expression (11) for the Landau free energy $F_L(\eta)$ gets a form

$$e^{\frac{F-F_L(\eta)}{T}} = \left(\frac{T}{2\pi}\right)^s \int du\, e^{\frac{\sum_a iu_a\eta_a}{T}} \mathbf{F}(iu) = \left(\frac{T}{2\pi}\right)^s \mathbf{F}(T\frac{\partial}{\partial\eta}) \int du\, e^{\frac{\sum_a iu_a\eta_a}{T}} = \mathbf{F}(T\frac{\partial}{\partial\eta})\delta(\eta),$$

i.e. such a representation for a nonequilibrium free energy is true

$$e^{\frac{F-F_L(\eta)}{T}} = \mathbf{F}(T\frac{\partial}{\partial\eta})\delta(\eta). \tag{16}$$

Here the formula is taken into account

$$\mathrm{f}(k)e^{ikx} = \mathrm{f}(-i\partial/\partial x)e^{ikx}, \tag{17}$$

that can be easily proved by the function $\mathrm{f}(-i\partial/\partial x)$ expansion in Taylor series. The generating function of average values (12) is related to the generating function $\mathbf{G}(h)$ of the correction function $\langle\hat\eta_{a_1}...\hat\eta_{a_n}\rangle$ with a known formula

$$\mathbf{F}(u) = e^{-\frac{\sum_a u_a\eta_a^{\mathrm{eq}}}{T} + \mathbf{G}(u)} \qquad (\eta_a^{\mathrm{eq}} \equiv \mathrm{Sp}\, w\hat\eta_a) \tag{18}$$

(η_a^{eq} is an equilibrium value of the order parameter; see, for example, [9]). For the generation function $\mathbf{G}(h)$ such standard identities are true

$$\mathbf{G}(u) = \sum_{n=2}^{\infty} \frac{(-1)^n}{T^n n!} \sum_{a_1...a_n} u_{a_1}...u_{a_n} \langle\hat\eta_{a_1}...\hat\eta_{a_n}\rangle, \qquad \left.\frac{\partial^s \mathbf{G}(u)}{\partial u_{a_1}...\partial u_{a_s}}\right|_{u=0} = \frac{(-1)^n}{T^n}\langle\hat\eta_{a_1}...\hat\eta_{a_s}\rangle. \tag{19}$$

With taking into account (18), the formula (16) for the Landau free energy $F_L(\eta)$ can be consistently presented in the form

$$e^{\frac{F-F_L(\eta)}{T}} = e^{-\sum_a \eta_a^{\mathrm{eq}}\frac{\partial}{\partial\eta_a} + \mathbf{G}(T\frac{\partial}{\partial\eta})}\delta(\eta) = e^{\mathbf{G}(T\frac{\partial}{\partial\eta})}\delta(\eta-\eta^{\mathrm{eq}}) =$$

$$= \frac{1}{(2\pi)^s} e^{\mathbf{G}(T\frac{\partial}{\partial\eta})} \int du e^{iu(\eta-\eta^{\mathrm{eq}})} = \frac{1}{(2\pi)^s} \int du e^{\mathbf{G}(iTu)} e^{iu(\eta-\eta^{\mathrm{eq}})}.$$

In this case the relation

$$\mathrm{f}(x+a) = e^{a\frac{\partial}{\partial x}}\mathrm{f}(x), \tag{20}$$

was taken into account which is another form of writing the expansion of a function $\mathrm{f}(x+a)$ in Taylor series in powers of a.

So, the following final expression for the Landau free energy is given by the formula

$$e^{\frac{F-F_L(\eta)}{T}} = \frac{1}{(2\pi)^s}\int du e^{\mathbf{G}(iTu)} e^{\sum_a iu_a\delta\eta_a} \qquad (\delta\eta_a \equiv \eta_a - \eta_a^{\text{eq}}), \tag{21}$$

here according to (19),

$$\mathbf{G}(iTu) = \sum_{n=2}^{\infty}\frac{(-i)^n}{n!}\sum_{a_1\ldots a_n} u_{a_1}\ldots u_{a_n}\langle\hat{\eta}_{a_1}\ldots\hat{\eta}_{a_n}\rangle . \tag{22}$$

The integral included in (21) can be precisely calculated only if we restrict ourselves with quadratic form as the expression for $\mathbf{G}(iTu)$

$$\mathbf{G}_2(iTu) = -\frac{1}{2}\sum_{a,b} u_a u_b A_{ab}, \qquad A_{ab} \equiv \langle\hat{\eta}_a\hat{\eta}_b\rangle . \tag{23}$$

In this approximation we have

$$e^{\frac{F-F_L(\eta)}{T}} \simeq \frac{1}{(2\pi)^s}\int du e^{\mathbf{G}_2(iTu)} e^{\sum_a iu_a\delta\eta_a} = \frac{1}{[(2\pi)^s \det A]^{1/2}} e^{-\frac{1}{2}\sum_{a,b} A_{ab}^{-1}\delta\eta_a\delta\eta_b} \tag{24}$$

and the Landau free energy gets the form

$$F_L(\eta) \simeq F + \frac{T}{2}\ln[(2\pi)^s \det A] + \frac{T}{2}\sum_{a,b} A_{ab}^{-1}\delta\eta_a\delta\eta_b . \tag{25}$$

Such an approximation for nonequilibrium free energy can be called the Gaussian one.

For small $\delta\eta_a$ the integral (21) can be expanded in series in powers of $\delta\eta_a$

$$e^{\frac{F-F_L(\eta)}{T}} = A_0 + \sum_{n=1}^{\infty}\sum_{a_1\ldots a_n} A_{a_1\ldots a_n}\delta\eta_{a_1}\ldots\delta\eta_{a_n} \tag{26}$$

where

$$A_0 = \frac{1}{(2\pi)^s}\int du e^{\mathbf{G}(iTu)}, \qquad A_{a_1\ldots a_n} = \frac{(-i)^n}{(2\pi)^s n!}\int du e^{\mathbf{G}(iTu)} u_{a_1}\ldots u_{a_n} . \tag{27}$$

To obtain an explicit expression for the free energy, we should compute the logarithm of the series in (26). This problem is solved by the formula

$$\begin{aligned} &\ln[b_0 + b_1 x + b_2 x^2 + b_3 x^3 + b_4 x^4 + O(x^5)] = \\ &= \ln b_0 + \frac{b_1}{b_0}x + \left(\frac{b_2}{b_0} - \frac{b_1^2}{2b_0^2}\right)x^2 + \left(\frac{b_3}{b_0} - \frac{b_1 b_2}{b_0^2} + \frac{b_1^3}{3b_0^3}\right)x^3 + \\ &+ \left(\frac{b_4}{b_0} - \frac{b_2^2}{2b_0^2} - \frac{b_1 b_3}{b_0^2} + \frac{b_1^2 b_2}{b_0^3} - \frac{b_1^4}{4b_0^4}\right)x^4 + O(x^5), \end{aligned} \tag{28}$$

if we make the following substitution

$$x \to 1, \; b_0 \to A_0, \qquad b_n \to \sum_{a_1\ldots a_n} A_{a_1\ldots a_n}\delta\eta_{a_1}\ldots\delta\eta_{a_n} .$$

Thus, the problem of calculating Landau nonequilibrium free energy $F_L(\eta)$ is solved in the general form with accuracy up to contributions of the fourth order in deviations of the order parameter from its value in equilibrium in the absence of an external field $\delta\eta_a \equiv \eta_a - \eta_a^{\mathrm{eq}}$. The further concretization of the obtained results is possible only with the specification of the problem and taking into account the symmetry of the system that simplifies the result.

3. The Landau effective Hamiltonian of an isotropic magnetic system in the paramagnetic phase

Let consider the case of a magnetic isotropic system in the absence of an external magnetic field. In this case the components of the magnetic dipole moment vector of the system m_n play the role of the order parameters η_a in phase transition paramagnetic-ferromagnetic. Therefore, we set the problem of calculation of the nonequilibrium Landau free energy (the Landau effective Hamiltonian) of a spatially homogeneous paramagnetic with a small magnetization.

A microscopic value of a magnetic moment $\hat{m}_n$ changes sign at the time reversal but the Hamiltonian $\hat{H}$ is unchanged. So, the mean values (12) of products of an odd number of magnetic moments $\hat{m}_n$ are zero

$$\overline{\hat{m}_{n_1} ... \hat{m}_{n_{2s+1}}} = 0 . \tag{29}$$

At the same time, according to (14), (18), and (19), an equilibrium average m_{n0} and correlation functions of an odd number of moments are also zero

$$m_{n0} = 0 , \qquad \langle \hat{m}_{n_1} ... \hat{m}_{n_{2s+1}} \rangle = 0 . \tag{30}$$

Formulas (26) and (27) for the Landau free energy $F_L(m)$ take the form

$$e^{\frac{F - F_L(m)}{T}} = A_0 + \sum_{s=1}^{\infty} A_{n_1 ... n_{2s}} m_{n_1} ... m_{n_{2s}} ;$$
$$A_0 = \frac{1}{(2\pi)^3} \int d^3 u e^{\mathbf{G}(iTu)} , \qquad A_{n_1 ... n_{2s}} = \frac{(-1)^s}{(2\pi)^3 (2s)!} \int d^3 u e^{\mathbf{G}(iTu)} u_{n_1} ... u_{n_{2s}} \tag{31}$$

because under conditions (29) generating functions $\mathbf{F}(u)$ and $\mathbf{G}(u)$ are even functions of the vector u_n (here Einstein's rule is used in the first formula). In the case of an isotropic system, that is true for the paramagnetic phase, the first tensors $A_{n_1 ... n_{2s}}$ have a structure

$$A_0 = \frac{1}{(2\pi)^3} \int d^3 u e^{\mathbf{G}(iTu)} \equiv a , \qquad A_{lm} = -\frac{1}{(2\pi)^3 2!} \int d^3 u e^{\mathbf{G}(iTu)} u_l u_m \equiv b \delta_{lm} ,$$
$$A_{lmsq} = \frac{1}{(2\pi)^3 4!} \int d^3 u e^{\mathbf{G}(iTu)} u_l u_m u_s u_q \equiv \frac{c}{3} (\delta_{lm}\delta_{sq} + \delta_{ls}\delta_{mq} + \delta_{lq}\delta_{ms}) \tag{32}$$

and expression (31) for the Landau free energy gives

$$e^{\frac{F - F_L(m)}{T}} = a + bm^2 + cm^4 + ... \qquad (m^2 \equiv m_n m_n , \quad m^4 \equiv (m^2)^2). \tag{33}$$

The coefficients a, b, c, according to (33), are given by the formulas

$$a = \frac{1}{(2\pi)^3}\int d^3u e^{\mathbf{G}(iTu)}, \qquad b = -\frac{1}{(2\pi)^2 3!}\int d^3u e^{\mathbf{G}(iTu)} u^2, \qquad c = \frac{1}{(2\pi)^3 5!}\int d^3u e^{\mathbf{G}(iTu)} u^4 . \tag{34}$$

Now we put in formula (28)

$$b_0 = a, \quad b_1 = 0, \quad b_2 = b, \quad b_3 = 0, \quad b_4 = c$$

and therefore obtain such a summary expression for the Landau free energy in the form of a series in moment powers

$$F_L(m) = F - T\ln a - \frac{Tb}{a}m^2 + \frac{T(b^2 - 2ac)}{2a^2}m^4 + \ldots \tag{35}$$

This formula, taking into account (34), shows that the coefficient at m^2 is positive in accordance with the Landau theory of the phase transition paramagnetic–ferromagnetic [3].

The coefficients a, b, c in (35) are given by formulas (34) and expressed through the correlation functions $\langle \hat{m}_{n_1} \ldots \hat{m}_{n_s} \rangle$. Contributions of correlation functions of four or more moments can only approximately be taken into account. Really, the simplest correlation functions $\langle \hat{m}_{n_1} \ldots \hat{m}_{n_s} \rangle$ in the case of an isotropic system have the tensor structure

$$\langle \hat{m}_l \hat{m}_m \rangle \equiv b_0 \delta_{lm}, \quad \langle \hat{m}_l \hat{m}_m \hat{m}_s \hat{m}_q \rangle \equiv \frac{c_0}{3}(\delta_{lm}\delta_{sq} + \delta_{ls}\delta_{mq} + \delta_{lq}\delta_{ms}), \tag{36}$$

where in short (33) notations

$$b_0 = \frac{1}{3}\langle \hat{m}^2 \rangle, \qquad c_0 = \frac{1}{5}\langle \hat{m}^4 \rangle . \tag{37}$$

In this case, according to (19), the generating function takes the form

$$\mathbf{G}(u) = \frac{b_0}{2T^2}u^2 + \frac{c_0}{24T^4}u^4 + \ldots . \tag{38}$$

According to (34), the calculation of coefficients a, b, c in the expression for the free energy (35) is reduced to the calculation of integrals

$$a = \frac{1}{(2\pi)^3}\int d^3u e^{-\frac{b_0}{2}u^2 + \frac{c_0}{24}u^4 + \ldots}, \qquad b = -\frac{1}{(2\pi)^3 3!}\int d^3u\, u^2 e^{-\frac{b_0}{2}u^2 + \frac{c_0}{24}u^4 + \ldots}, \qquad c = \frac{1}{(2\pi)^3 5!}\int d^3u\, u^4 e^{-\frac{b_0}{2}u^2 + \frac{c_0}{24}u^4 + \ldots} . \tag{39}$$

It is clear from (39) that we can take into consideration the contributions of four and more moments only approximately. Neglecting all correlations $\langle m^{2s} \rangle$ with $s > 2$, we have for the coefficients a, b, c

$$a = \frac{1}{2\pi^2}\int_0^\infty du\, u^2 e^{-\frac{b_0}{2}u^2 + \frac{c_0}{24}u^4} = \frac{2^{1/2}}{\pi^2 b_0^{3/2}}\int_0^\infty d\upsilon\, \upsilon^2 e^{-\upsilon^2} e^{\frac{\alpha}{6}\upsilon^4} s,$$

$$b = -\frac{1}{2\pi^2 3!}\int_0^\infty du\, u^4 e^{-\frac{b_0}{2}u^2 + \frac{c_0}{24}u^4} = -\frac{2^{1/2}}{3\pi^2 b_0^{5/2}}\int_0^\infty d\upsilon\, \upsilon^4 e^{-\upsilon^2} e^{\frac{\alpha}{6}\upsilon^4}, \qquad (40)$$

$$c = \frac{1}{2\pi^2 5!}\int_0^\infty du\, u^6 e^{-\frac{b_0}{2}u^2 + \frac{c_0}{24}u^4} = \frac{1}{2^{1/2} 15\pi^2 b_0^{7/2}}\int_0^\infty d\upsilon\, \upsilon^6 e^{-\upsilon^2} e^{\frac{\alpha}{6}\upsilon^4}$$

($\alpha \equiv c_0 / b_0^2$). Further calculation can be done assuming that the correlation function $\langle \hat{m}^4 \rangle$ is small. In this case, according to (37), the value c_0 is small and the dimensionless small parameter of the theory is α. Thus,

$$a = \frac{2^{1/2}}{\pi^2 b_0^{3/2}}\int_0^\infty d\upsilon\, \upsilon^2 e^{-\upsilon^2}(1 + \frac{\alpha}{6}\upsilon^4) + O(\alpha^2),$$

$$b = -\frac{2^{1/2}}{3\pi^2 b_0^{5/2}}\int_0^\infty d\upsilon\, \upsilon^4 e^{-\upsilon^2}(1 + \frac{\alpha}{6}\upsilon^4) + O(\alpha^2), \qquad (41)$$

$$c = \frac{1}{2^{1/2} 15\pi^2 b_0^{7/2}}\int_0^\infty d\upsilon\, \upsilon^6 e^{-\upsilon^2}(1 + \frac{\alpha}{6}\upsilon^4) + O(\alpha^2).$$

If the integral value is taken into account

$$\int_0^\infty d\upsilon\, \upsilon^{2s} e^{-\upsilon^2} = \Gamma(s + 1/2)/2, \qquad (42)$$

we have

$$a = \frac{1}{2^{3/2}\pi^{3/2} b_0^{3/2}}\left[1 + \frac{5}{2^3}\alpha + O(\alpha^2)\right], \qquad b = -\frac{1}{2^{5/2}\pi^{3/2} b_0^{5/2}}\left[1 + \frac{35}{24}\alpha + O(\alpha^2)\right],$$

$$c = \frac{1}{2^{9/2}\pi^{3/2} b_0^{7/2}}\left[1 + \frac{21}{2^3}\alpha + O(\alpha^2)\right]. \qquad (43)$$

Taking into account these expressions, the free energy $F_L(m)$ (35) also need to be calculated in the form of a series in α powers that gives

$$F_L(m) = F + \frac{3T}{2}\ln(2\pi b_0) - \frac{5T}{8}\alpha + \frac{T}{2b_0}(1 + \frac{5}{6}\alpha)m^2 - \frac{T}{24 b_0^2}\alpha m^4. \qquad (44)$$

Proceeding from the expressions (37) for the coefficients b_0, c_0, the Landau free energy (the Landau effective Hamiltonian) can be written in such a final form

$$F_L(m) = F + \frac{3T}{2}\left(\ln\frac{2\pi\langle\hat{m}^2\rangle}{3} - \frac{3}{4}\frac{\langle\hat{m}^4\rangle}{\langle\hat{m}^2\rangle^2}\right) + \\ + \frac{3T}{2\langle\hat{m}^2\rangle}\left(1 + \frac{3}{2}\frac{\langle\hat{m}^4\rangle}{\langle\hat{m}^2\rangle^2}\right)m^2 - \frac{27T}{40}\frac{\langle\hat{m}^4\rangle}{\langle\hat{m}^2\rangle^4}m^4 \quad (45)$$

This expression has the form of a series in powers of small magnetic moment m_l written with the accuracy up to the fourth order inclusive. The coefficients of this series are calculated neglecting by the correlations $\langle\hat{m}^{2s}\rangle$ with $s > 2$ in the perturbation theory in the parameter α that assumes the fulfillment of the inequality

$$\alpha = c_0 / b_0^2 = 9\langle\hat{m}^4\rangle / 5\langle\hat{m}^2\rangle^2 \ll 1. \quad (46)$$

Formula (45) gives the Landau free energy (the Landau effective Hamiltonian) in the paramagnetic phase. In accordance with his theory of phase transitions, the sign of the coefficient at m^2 is positive. In contradiction with the Landau theory coefficient at m^4, has negative sign. Perhaps, this is a consequence of discussible assumption that correlations of the four magnetic moments are small near the transition point paramagnetic–ferromagnetic.

Let us compare the Landau nonequilibrium free energy (45) of a magnetic in paramagnetic phase with the corresponding expression for the Landau–Leontovich nonequilibrium free energy

$$F_{LL}(m) = F_0 + \frac{3}{2}\frac{T}{\langle\hat{m}^2\rangle}m^2 - \frac{27}{40}\frac{T\langle\hat{m}^4\rangle}{\langle\hat{m}^2\rangle^4}m^4 \quad (47)$$

obtained in our paper [6]. This formula gives truncated series of expansion $F_{LL}(m)$ in powers of m neglecting terms of the order m^{2s} with $s > 2$. It is seen a full match of both expressions for nonequilibrium free energy at the condition (46).

4. Conclusions

We have realized the Landau definition of the effective Hamiltonian (the nonequilibrium free energy) of a system in a microscopic theory. This definition is formulated in such a way that the Boltzmann principle is an exact result and effective Hamiltonian determines the total equilibrium free energy. The developed theory is applied to a magnetic in the paramagnetic phase. The result is compared with the Landau–Leontovich nonequilibrium free energy obtained by us early in [6]. A complete coincidence of the results is seen in the limit of small magnetic moment correlation functions of the fourth order.

The final expression for the Landau effective Hamiltonian of an isotropic magnetic system in the paramagnetic phase shows that the coefficient at the second power of the magnetic moment is positive and the coefficient at the fourth power is negative at an arbitrary temperature. The positivity of the coefficient for the second power is in agreement with the Landau theory of phase transitions of the second kind. However, the negativity of the coefficient at the fourth power contradicts to standard theory. In this case the sixth in magnetic moment terms should be taken into account in the theory [7].

The obtained general results are specified for the phase transition between the ferromagnetic and paramagnetic phases. In the calculation of nonequilibrium free energy in the paramagnetic phase the system is considered as an isotropic one, i.e. its states are rotationally invariant. In its physical content, the phase transition ferromagnetic–paramagnetic is accompanied by the mentioned symmetry breaking and this should be taken into account when investigating the situation in the ferromagnetic phase. This is planned to be done in the future.

The developed theory can be generalized for the case in which magnetization of the system $M_n(x)$ is considered as the order parameter by the substitution in our general formulas (26), (27)

$$\eta_a \to M_n(x), \qquad \sum_a ... \to \sum_n \int d^3x ..., \qquad u_a \to u_n(x)$$

that allows to account the fluctuation effects in the theory (see, for example, [7, 9]).

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