RANDOM PHASE APPROXIMATION FOR THE BLINC-DE GENNES MODEL FOR HYDROGEN-BONDED FERROELECTRICS

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The Blinc-De Gennes model is considered in the framework of the Random Phase Approximation (RPA) taking into account the conditions following from the commutation relations and the averaged equations of motion for the spin operators. In this way conditions for the consistency of the RPA are obtained. These conditions are satisfied in the case of high and low temperatures, and for $T \approx T_c$ if $\sigma_0 = \Gamma/I(0) \lesssim 1/2$. For $T \approx T_c$ and $2\sigma_0 \ll 1$ the RPA breaks down.

1. Introduction

In this paper we consider the random phase approximation (RPA) for the Blinc-De Gennes model [1–7] for hydrogen-bonded ferroelectrics described by the Hamiltonian

$$H = -\Gamma \sum_i \hat{S}_i^x - \mathscr{E} \sum_i \hat{S}_i^z - \tfrac{1}{2} \sum_{i,j} I_{ij} \hat{S}_i^z \hat{S}_j^z . \tag{1}$$

The spin operator $\hat{\boldsymbol{S}}$ describes the states of the protons in the double-minimum potential wall (the eigenvalues correspond to the two possible equilibrium positions of the protons). The first term in (1) describes the tunnelling of the protons, Γ is the tunnelling frequency. The second term arises from a possible asymmetry of the potential wall *e. g.* due to the interaction with the heavy ions. The last term is the interaction between the protons. It is assumed that

$$I_{ij} = I_{ji} > 0, \; I_{ii} = 0. \tag{2}$$

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Compared to the real situation (consider *e. g.* KH_2PO_4) this model has to be extended by the inclusion of the interaction with the heavy ions which give rise to the polarization. Furthermore, for simplicity we consider a lattice with only one proton in the elementary cell.

The Green-function method and the RPA for the model (1) have been considered in the papers [8, 9], where the spectrum of the elementary excitations and the equation for the order parameter were obtained. However, in these papers difficulties arise in connection with the fulfilment of the thermally averaged conditions:

$$\langle(\hat{S}_i^{\alpha})^2\rangle = \tfrac{1}{4},$$

$$\langle\hat{S}_i^{\alpha_1}\hat{S}_i^{\alpha_2}\rangle = \frac{i}{2}\langle\hat{S}_i^{\alpha_3}\rangle, \tag{3}$$

($\alpha_1\alpha_2\alpha_3$ — cyclic indices) holding for $S = 1/2$. The equation for the order parameter is obtained in [8–11] from one (or a combination) of the conditions (3). The resulting equations have different forms depending on the chosen condition.

It is the aim of the present paper to discuss the RPA for the model (1) taking into account all the six conditions (3) and also the thermally averaged equations of motion for the spin operators

$$\left\langle i\frac{\partial}{\partial t}\hat{S}_i^{\alpha}\right\rangle = 0. \tag{4}$$

We show that the relations (3) and (4) may be satisfied in the framework of the RPA provided that some condition (see Eq. (42) and (44) below) is fulfilled. This condition, restricting the applicability of the RPA is discussed simultaneously with the equation for the order parameter.

The general method of this paper may be also interesting from the point of view of the theory of anisotropic ferromagnets.

2. Calculation of the Green functions and the correlation functions

To obtain a compact formulation we introduce the spin operators S_i^{α} in a rotated system of coordinates

$$\hat{S}_i^{\nu} = (\boldsymbol{a}^{\nu}\cdot\boldsymbol{S}_i). \tag{5}$$

The unit vectors $\boldsymbol{a}^{\nu}$, which belong to the old system of coordinates obey the conditions

$$\boldsymbol{a}^{\nu_1}\times\boldsymbol{a}^{\nu_2} = \boldsymbol{a}^{\nu_3}. \tag{6}$$

We denote quantities in the old system of coordinates ($a^{\nu\alpha} = \delta_{\nu\alpha}$) by the symbol $\wedge$.

In the new system of coordinates the Hamiltonian (1) takes the form

$$H = -\Gamma\sum_i(\boldsymbol{a}^x\cdot\boldsymbol{S}_i) - \mathscr{E}\sum_i(\boldsymbol{a}^z\cdot\boldsymbol{S}_i) - \\ -\tfrac{1}{2}\sum_{i,j}I_{ij}(\boldsymbol{a}^z\cdot\boldsymbol{S}_i)(\boldsymbol{a}^z\cdot\boldsymbol{S}_j). \tag{7}$$

The Hamiltonian (7) leads to the equations of motion

$$i\frac{\partial}{\partial t}\boldsymbol{S}_l = -i\Gamma(\boldsymbol{a}^x \times \boldsymbol{S}_l) - i\mathscr{E}(\boldsymbol{a}^z \times \boldsymbol{S}_l) -$$

$$-i\sum_j I_{lj}(\boldsymbol{a}^z \times \boldsymbol{S}_l)\,(\boldsymbol{a}^z \cdot \boldsymbol{S}_j). \tag{8}$$

We use the Matsubara-type Green functions defined by

$$G_{lm}^{\alpha_1\alpha_2}(t_1 - t_2) = \frac{1}{i}\langle T(S_l^{\alpha_1}(t_1) - \langle S^{\alpha_1}\rangle)\,(S_m^{\alpha_2}(t_2) - \langle S^{\alpha_2}\rangle)\rangle. \tag{9}$$

In the framework of the RPA these Green functions obey the equations of motion

$$i\frac{\partial}{\partial t_1}G_{lm}^{\alpha_1\gamma}(t_1 - t_2) = \delta_{lm}\delta(t_1 - t_2)\,\langle[S_l^{\alpha_1}, S_l^{\gamma}]\rangle -$$

$$-i[E^{\alpha_2}G_{lm}^{\alpha_3\gamma}(t_1 - t_2) - E^{\alpha_3}G_{lm}^{\alpha_2\gamma}(t_1 - t_2)] -$$

$$-i(\boldsymbol{a}^z \times \langle \boldsymbol{S}\rangle)_{\alpha_1}\sum_{j\beta} I_{lj}a^{z\beta}G_{jm}^{\beta\gamma}(t_1 - t_2), \tag{10}$$

where

$$\boldsymbol{E} = \Gamma\boldsymbol{a}^x + \mathscr{E}\boldsymbol{a}^z + I(0)\,\langle\hat{S}^z\rangle\boldsymbol{a}^z \tag{11}$$

is the effective field in the molecular field approximation (MFA), and $\sum_j I_{jl} = I(0)$.

In (10) we have neglected the term with

$$\frac{1}{i}\langle T(S_l^{\alpha}(t_1) - \langle S^{\alpha}\rangle)\,(S_j^{\beta}(t_1) - \langle S^{\beta}\rangle)\,(S_m^{\gamma}(t_2) - \langle S^{\gamma}\rangle)\rangle,$$

because the decoupling procedure of the RPA leads to a vanishing result. The neglection of the last term in (10) corresponds to the MFA.

By Fourier transformation of (10) we obtain

$$\omega_n G^{\alpha_1\gamma}(\boldsymbol{k}, \omega_n) = \langle[S^{\alpha_1}, S^{\gamma}]\rangle -$$

$$-i[E^{\alpha_1}G^{\alpha_3\gamma}(\boldsymbol{k}, \omega_n) - E^{\alpha_3}G^{\alpha_2\gamma}(\boldsymbol{k}, \omega_n)] -$$

$$-i(\boldsymbol{a}^z \times \langle \boldsymbol{S}\rangle)_{\alpha_1}I(\boldsymbol{k})\sum_{\beta} a^{z\beta}G^{\beta\gamma}(\boldsymbol{k}, \omega_n), \tag{12}$$

where $\omega_n = 2\pi i n/\beta$.

To solve equations (12) we make the "ansatz":

$$G^{\alpha_1\gamma}(\boldsymbol{k}, \omega_n) = \frac{\omega_n}{\omega_n^2 - \omega^2(\boldsymbol{k})}\,\langle[S^{\alpha_1}, S^{\gamma}]\rangle +$$

$$+\frac{1}{\omega_n^2 - \omega^2(\boldsymbol{k})}\,g^{\alpha_1\gamma}(\boldsymbol{k}) - \beta\delta_{\omega_n,0}f^{\alpha_1\gamma}(\boldsymbol{k}). \tag{13}$$

Because $G^{\alpha_1\gamma}(\boldsymbol{k}, \omega_n)$ has to be invariant with respect to the transformation $\alpha_1 \leftrightarrow \gamma$, $\omega_n \to -\omega_n$, $\boldsymbol{k} \to -\boldsymbol{k}$, it follows that $g^{\alpha_1\gamma}(\boldsymbol{k}) = g^{\gamma\alpha_1}(\boldsymbol{k})$ and $f^{\alpha_1\gamma}(\boldsymbol{k}) = f^{\gamma\alpha_1}(\boldsymbol{k})$. (The change $\boldsymbol{k} \to -\boldsymbol{k}$ has no influence, because $\boldsymbol{k}$ enters the equations (12) only through $I(\boldsymbol{k}) = I(-\boldsymbol{k})$.)

By substituting (13) into (12) and considering separately the cases where $\omega_n \neq 0$ and $\omega_n = 0$, we obtain the following equations for $g^{\alpha_1\gamma}(\boldsymbol{k})$, $\omega(\boldsymbol{k})$ and $f^{\alpha_1\gamma}(\boldsymbol{k})$:

$$g^{\alpha\beta}(\boldsymbol{k}) = \delta_{\alpha\beta}\boldsymbol{E}\cdot\langle\boldsymbol{S}\rangle - E^{\alpha}\langle S^{\beta}\rangle - \\ - I(k)\,(\boldsymbol{a}^z\times\langle\boldsymbol{S}\rangle)_{\alpha}\,(\boldsymbol{a}^z\times\langle\boldsymbol{S}\rangle)_{\beta}, \tag{14}$$

$$\omega^2(\boldsymbol{k})\,\langle[S^{\alpha_1}, S^{\gamma}]\rangle = -iE^{\alpha_2}g^{\alpha_3\gamma}(\boldsymbol{k}) + iE^{\alpha_3}g^{\alpha_2\gamma}(\boldsymbol{k}) - \\ - i(\boldsymbol{a}^z\times\langle\boldsymbol{S}\rangle)_{\alpha_1}I(\boldsymbol{k})\sum_{\mu}a^{z\mu}g^{\mu\gamma}(\boldsymbol{k}), \tag{15}$$

$$E^{\alpha_2}f^{\alpha_3\gamma}(\boldsymbol{k}) - E^{\alpha_3}f^{\alpha_2\gamma}(\boldsymbol{k}) + \\ + (\boldsymbol{a}^z\times\langle\boldsymbol{S}\rangle)_{\alpha_1}I(\boldsymbol{k})\sum_{\mu}a^{z\mu}f^{\mu\gamma}(\boldsymbol{k}) = 0. \tag{16}$$

The symmetry property of the $g^{\alpha_1\gamma}(\boldsymbol{k})$ leads to the condition

$$(\boldsymbol{E}\times\langle\boldsymbol{S}\rangle) = 0, \tag{17}$$

which takes in the old system of coordinates the form

$$\langle\hat{S}^y\rangle = 0, \tag{18}$$

$$\Gamma\langle\hat{S}^z\rangle - \langle\hat{S}^x\rangle\,(\mathscr{E} + I(0)\,\langle\hat{S}^z\rangle) = 0. \tag{19}$$

Equation (19) showing the possibility of the phase transition was already obtained in [4–10][1].

In the case where $\mathscr{E} = 0$ equation (19) has two solutions:

$$\langle\hat{S}^z\rangle = 0 \text{ for } T > T_c \tag{20}$$

and

$$\langle\hat{S}^z\rangle \neq 0,\ \langle\hat{S}^x\rangle = \Gamma/I(0) \equiv \sigma_0 \text{ for } T < T_c \tag{21}$$

(T_c is the temperature of the Curie point). We introduce the angle θ between the x-axis and the vector $\langle\boldsymbol{S}\rangle$ by

$$\theta = 0 \text{ for } T > T_c$$

and

$$\sigma^2 = \langle\boldsymbol{S}\rangle^2,\ \cos\theta = \sigma_0/\sigma \text{ for } T < T_c, \tag{22}$$

and note the relations

$$\langle\hat{S}^z\rangle = \sigma\sin\theta,$$

$$\boldsymbol{a}^z\times\langle\boldsymbol{S}\rangle = \boldsymbol{a}^y\sigma\cos\theta,$$

$$\boldsymbol{E} = \frac{\langle\boldsymbol{S}\rangle}{\sigma}\cdot\frac{\Gamma}{\cos\theta}. \tag{23}$$

[1] The same condition results in the MFA, because the last term in (14) is symmetrical.

Using (17) we get from (15)

$$\omega^2(\boldsymbol{k}) = \boldsymbol{E}\cdot\{\boldsymbol{E}+I(\boldsymbol{k})\boldsymbol{a}^z\times(\boldsymbol{a}^z\times\langle\boldsymbol{S}\rangle)\} =$$
$$=\Gamma(\Gamma-I(\boldsymbol{k})\langle\hat{S}^x\rangle)+(\mathscr{E}+I(0)\langle\hat{S}^z\rangle)^2. \tag{24}$$

The spectrum (24) of the elementary excitations was already found in [2, 4–10].

The Green functions for $\omega_n = 0$ are not determined uniquely, because the determinant of the homogeneous system (16) for the functions $f^{\alpha\beta}(\boldsymbol{k})$ vanishes. This effect was already noticed by Pytte and Thomas [7], who have calculated the Green functions for $\omega_n = 0$ in MFA with the help of the relation

$$G^{\alpha\beta}(\boldsymbol{k}, \omega_n = 0) = -\chi^{\alpha\beta}(\boldsymbol{k}), \tag{25}$$

where $\chi^{\alpha\beta}(k)$ is the isothermal susceptibility. It is of course possible to extend this calculation to the RPA. However, in the present paper we restrict ourselves to the information, which can be obtained from the system (16). In the old system of coordinates equation (16) takes the form

$$\hat{f}^{yy}(\boldsymbol{k}) = 0, \tag{26}$$

$$(\sigma\cos\theta\cdot I(\boldsymbol{k})-\Gamma)\hat{f}^{zy}(\boldsymbol{k})+I(0)\langle\hat{S}^z\rangle\hat{f}^{xy}(\boldsymbol{k}) = 0. \tag{27}$$

Above the Curie point Eq. (27) gives

$$\hat{f}^{zy}(\boldsymbol{k}) = 0 \text{ for } T > T_c. \tag{28}$$

We now calculate the correlation functions for the spin operators. Using the formula

$$\langle S_l^\alpha(t)S_m^\beta(t)\rangle_k = -\frac{1}{\beta}\sum_{\omega_n} G^{\alpha\beta}(\boldsymbol{k}, \omega_n)e^{-i\omega_n\tau}\Big|_{\tau\to-i0} +$$
$$+N\delta_{k,0}\langle S^\alpha\rangle\langle S^\beta\rangle =$$
$$= iP\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{e^{\beta\omega/2}}{e^{\beta\omega/2}-e^{-\beta\omega/2}}\{G^{\alpha\beta}(\boldsymbol{k}, \omega+i\varepsilon)-G^{\alpha\beta}(\boldsymbol{k}, \omega-i\varepsilon)\}-$$
$$-\frac{1}{\beta}\left\{G^{\alpha\beta}(\boldsymbol{k}, \omega_n = 0)-\frac{1}{2}(G^{\alpha\beta}(\boldsymbol{k}, i\varepsilon)+G^{\alpha\beta}(\boldsymbol{k}, -i\varepsilon))\right\} +$$
$$+N\delta_{k,0}\langle S^\alpha\rangle\langle S^\beta\rangle, \tag{29}$$

and (13) and (14) we obtain

$$\langle S_l^\alpha(t)S_m^\beta(t)\rangle_k = \tfrac{1}{2}\langle[S^\alpha, S^\beta]\rangle +$$
$$+\{\delta_{\alpha\beta}(\boldsymbol{E}\cdot\langle\boldsymbol{S}\rangle)-E^\alpha\langle S^\beta\rangle-I(\boldsymbol{k})(\boldsymbol{a}^z\times\langle\boldsymbol{S}\rangle)_\alpha(\boldsymbol{a}^z\times\langle\boldsymbol{S}\rangle)_\beta\}\times$$
$$\times\frac{1}{2\omega(\boldsymbol{k})}\operatorname{cth}\frac{\beta\omega(\boldsymbol{k})}{2} +$$
$$+N\delta_{k,0}\langle S^\alpha\rangle\langle S^\beta\rangle+f^{\alpha\beta}(\boldsymbol{k}). \tag{30}$$

3. *The averaged equations of motion and the conditions for* $S = 1/2$

We now consider the thermally averaged equations of motion (8). These equations coincide of course with the condition for a vanishing variation of the free energy with respect to a small rotation of the system of coordinates

$$\boldsymbol{a}^{\nu_1} \to \boldsymbol{a}^{\nu_1} + \xi^{\nu_2}\boldsymbol{a}^{\nu_3} - \xi^{\nu_3}\boldsymbol{a}^{\nu_2}, \tag{31}$$

where the independent infinitesimal angles ξ^ν correspond to rotations around the axes $\boldsymbol{a}^\nu$. In fact we have

$$0 = \frac{\partial F}{\partial \xi^\nu} = \left\langle \frac{\partial H}{\partial \xi^\nu} \right\rangle = -iN\boldsymbol{a}^\nu \langle [\boldsymbol{S}_l, H] \rangle, \tag{32}$$

because a rotation of the $\boldsymbol{a}^\nu$ may be substituted by the inverse rotation of the operators $\boldsymbol{S}_l$.

Using (17) and (30) we write the averaged equations of motion (8) in the form

$$0 = \left\langle \frac{\partial}{\partial t} \boldsymbol{S}_l(t) \right\rangle = I(0)\, \langle \hat{S}^z \rangle \boldsymbol{a}^y \langle \hat{S}^x \rangle -$$

$$- \frac{1}{N} \sum_k I(\boldsymbol{k})\, \langle (\boldsymbol{a}^z \times \boldsymbol{S}_l(t))\, (\boldsymbol{a}^z \cdot \boldsymbol{S}_j(t)) \rangle_k. \tag{33}$$

Equation (30) gives for the correlation function

$$- \frac{1}{N} \sum_k I(\boldsymbol{k})\, \langle (\boldsymbol{a}^z \times \boldsymbol{S}_l(t))\, (\boldsymbol{a}^z \cdot \boldsymbol{S}_j(t)) \rangle_k =$$

$$= -I(0)\, \langle \hat{S}^z \rangle\, \langle \hat{S}^x \rangle \boldsymbol{a}^y -$$

$$- \boldsymbol{a}^y \Gamma \langle \hat{S}^z \rangle \frac{1}{N} \sum_k \frac{I(\boldsymbol{k})}{2\omega(\boldsymbol{k})} \operatorname{cth} \frac{\beta\omega(\boldsymbol{k})}{2} -$$

$$- \boldsymbol{a}^y \frac{1}{N} \sum_k I(\boldsymbol{k}) f^{xz}(\boldsymbol{k}). \tag{34}$$

The first terms on the right-hand sides of (33) and (34) cancel out. Above the Curie point all terms on the right-hand side of (33) vanish, as can be seen from equations (20) nad (28), so that (33) is satisfied. Below the Curie point we have to require that the first term on the right-hand side of (34) gives the main contribution to the correlation function.

We now consider the condition (3) following from the commutation relation for $S = 1/2$ in the old system of coordinates (the conditions (3) are covariant with respect to

the transformation (5)). From (30), using also (23), we obtain

$$\langle(\hat{S}_l^x)^2\rangle = \frac{\Gamma\sigma \sin^2\theta}{\cos\theta}\sum_1 + \sigma^2\cos^2\theta + \hat{f}_0^{xx} = \frac{1}{4}, \tag{35}$$

$$\langle(\hat{S}_l^y)^2\rangle = \frac{\Gamma\sigma}{\cos\theta}\sum_1 - \sigma^2\cos^2\theta\sum_2 = \frac{1}{4}, \tag{36}$$

$$\langle(\hat{S}_l^z)^2\rangle = \Gamma\sigma\cos\theta\sum_1 + \sigma^2\sin^2\theta + \hat{f}_0^{zz} = \tfrac{1}{4}, \tag{37}$$

$$\langle\hat{S}_l^x\hat{S}_l^y\rangle = \frac{i}{2}\langle\hat{S}_l^z\rangle, \tag{38}$$

$$\langle\hat{S}_l^y\hat{S}_l^z\rangle = \frac{i}{2}\langle\hat{S}_l^x\rangle, \tag{39}$$

$$\langle\hat{S}_l^z\hat{S}_l^x\rangle = -\Gamma\sigma\sin\theta\sum_1 + \sigma^2\sin\theta\cos\theta + \hat{f}_0^{zx} = 0, \tag{40}$$

where

$$\sum_1 = \frac{1}{N}\sum_k \frac{1}{2\omega(\boldsymbol{k})}\operatorname{cth}\frac{\beta\omega(\boldsymbol{k})}{2},$$

$$\sum_2 = \frac{1}{N}\sum_k \frac{I(\boldsymbol{k})}{2\omega(\boldsymbol{k})}\operatorname{cth}\frac{\beta\omega(\boldsymbol{k})}{2},$$

$$\hat{f}_0^{\alpha\beta} = \frac{1}{N}\sum_k \hat{f}^{\alpha\beta}(\boldsymbol{k}). \tag{41}$$

The conditions (38) and (39) already have the right form. $\hat{f}_0^{yy} = 0$ because of the particular role of the xz-plane in the Hamiltonian (1), so that condition (36) leads immediately to an equation for the order parameter σ. We censider the other conditions above and below the Curie point separately.

(*i*) Above the Curie point

From the condition (37) we find a second equation for the order parameter and the requirement of compatibility with (36) leads to the condition

$$\sigma^2|\Sigma_2| \ll \tfrac{1}{4} \tag{42}$$

restricting the applicability of the RPA. The equation for the order parameter is

$$\Gamma\sigma\Sigma_1 = \tfrac{1}{4}. \tag{43}$$

The condition (40) is satisfied and condition (35) determines[2] $\hat{f}_0^{xx}$. Furthermore, the averaged equations of motion (33) are satisfied above the Curie point.

[2] It is necessary to remark that independent calculation of $\hat{f}_0^{xx}$ with the help of (25) may lead to further restriction of the RPA besides (42).

(*ii*) Below the Curie point

Below the Curie point, where $\cos\theta = \sigma_0/\sigma$, all the conditions (35)–(40) can be satisfied. However, the averaged equations of motion (33) can be satisfied only approximately (as was already remarked below equation (34)). With the help of (27) and (35), (36), (40) we obtain the condition

$$|\sum_2| \ll \tfrac{1}{2}. \tag{44}$$

Taking into account (44), the equation (36) for the order parameter σ can be written in the form

$$\frac{\Gamma\sigma^2}{\sigma_0} \cdot \sum_1 = \frac{1}{4}. \tag{45}$$

4. Discussion

The above considerations show that the conditions obtained from the thermally averaged commutation relations and from the averaged equation of motion can be satisfied only approximately in the framework of the RPA. It should be noted that all the equations for the order parameter σ which have been derived in the papers [8–11] differ by terms which can be neglected according to our conditions (42) and (44).

In explicit we obtain for the condition (42) (above the Curie point)

$$\frac{\sigma^2}{2\sigma_0 N}\left|\sum_k \frac{\gamma_k}{\sqrt{1-\frac{\sigma}{\sigma_0}\gamma_k}} \operatorname{cth}\frac{\beta\Gamma}{2}\sqrt{1-\frac{\sigma}{\sigma_0}\gamma_k}\right| \ll \frac{1}{4} \tag{46}$$

and for the condition (44) (below the Curie point)

$$\frac{1}{2\sigma N}\left|\sum_k \frac{\gamma_k}{\sqrt{1-\left(\frac{\sigma_0}{\sigma}\right)^2\gamma_k}} \operatorname{cth}\frac{\beta\sigma I(0)}{2}\sqrt{1-\left(\frac{\sigma_0}{\sigma}\right)^2\gamma_k}\right| \ll \frac{1}{2}, \tag{47}$$

where

$$\gamma_k = I(\boldsymbol{k})/I(0).$$

(*i*) High temperatures $T \gg T_c$.

The equation for the order parameter (43) has the solution $\sigma \approx \Gamma/4k_BT$. The left-hand side of the condition (46) takes the form $z^{-1}(I(0)/k_BT)^2$ (we consider only interactions between nearest neighbours, z being the number of nearest neighbours), and is small in comparison with 1/4 for sufficiently high T and z. Therefore, the condition of applicability of the RPA is satisfied.

(*ii*) Low temperatures $T \ll T_c$.

For $2\sigma_0 \ll 1$ the equation for the order parameter has the solution $2\sigma \approx 1$. The left-hand side of the inequality (47) is equal to $(2\sigma_0)^2/2z$, and therefore small in comparison with 1/2.

For $2\sigma_0 \lesssim 1/a_1$, where[3] [12]

$$a_1 = \frac{1}{N}\sum_k \frac{1}{\sqrt{1-\gamma_k}} = \begin{cases} 1.111 \text{ for } sc \text{ lattice} \\ 1.084 \text{ for } bcc \text{ lattice,} \end{cases}$$

the equation for the order parameter has the solution $2\sigma \approx 1/a_1$, and the left-hand side of the condition (47) is of the order of

$$a_1(a_1 - b_1) \approx 0.1,$$

where [12]

$$b_1 = \frac{1}{N}\sum_k \sqrt{1-\gamma_k} = \begin{cases} 0.975 \text{ for } sc \text{ lattice} \\ 0.981 \text{ for } bcc \text{ lattice.} \end{cases}$$

Therefore, the condition of the applicability of the RPA is not very well satisfied in this case.

(*iii*) Vicinity of the Curie temperature $T \approx T_c$.

In this case we have $\sigma \approx \sigma_0$. The two conditions (42) and (44) are equivalent for $2\sigma_0 \approx 1$, but different for $2\sigma_0 \ll 1$.

For $2\sigma_0 \ll 1$ the condition is only satisfied approximately above the Curie point (the left-hand side of (46) is of the order of $1/12 \div 1/15$), below the Curie point the left--hand side of (47) is of the order of $1/3(2\sigma_0)^2$ and the RPA breaks down.

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[3] We remark that the restriction $2\sigma_0 < 1/a_1$ is the condition for a positive solution for the Curie temperature T_c.