JOURNAL OF EXPERIMENTAL AND THEORETICAL PHYSICS, 2024, Vol. 165, No. 3, pp. 390–397

ORDER, DISORDER AND PHASE TRANSITIONS IN CONDENSED MEDIA

FERROMAGNETIC ORDER IN VAN-DER WAALS COMPOUND Fe_3GeTe_2

© 2024 V.V. Men`shenin*

Federal State Budgetary Institution of Science
M.N. Mikheev Institute of Metal Physics
Ural Branch of the Russian Academy of Sciences
620108, Yekaterinburg, Russia

**e-mail: menshenin@imp.uran.ru*

Received August 01, 2023
Revised September 07, 2023
Accepted September 07, 2023

Abstract. The phase transition from the paramagnetic to the ferromagnetic phase in a van der Waals volume Fe_3GeTe_2 compound was studied. A renormalization group approach was used, the action for which was constructed using group theoretical analysis to determine the irreducible representation of the spatial group responsible for this transition, in the case of magnetic moments localized on iron. It is shown that such a representation exists, which allows the orientation of magnetic moments along the c axis of the crystal. The influence of vacancies in one of the iron positions on this transition was considered using replica method by analogy with the description of frozen impurities. Power law of change magnetization was found near the transition taking into account the presence of vacancies. A condition has been determined when vacancies are pressure this transition. Possible influence of strong electron correlations and free electrons on the stability of the ferromagnetic phase was analyzed using the t–J model for non-degenerate electrons. In the generalized random phase approximation, the additional contribution of free electrons to the formation of long-range ferromagnetic order occurs through Pauli susceptibility gas of free electrons. The condition for the stability of the ferromagnetic state in this case was written out.

Keywords: *ferromagnetic order*, *van der Waals compound*, *phase transition*, *strong electron correlations*

DOI: 10.31857/S00444510240308e5

INTRODUCTION

Layered materials with weak interlayer bond of van der Waals are of increased interest. This is due to the fact that the properties of the system can be controlled by replacing one layer with another or reducing the dimension of the connection, highlighting single-layer components. Lowering the dimension leads to an increase in quantum effects, which can be useful in applications. An example of such a compound is iron dichalcogenide Fe_3GeTe_2. This compound is a metallic ferromagnet [1, 2, 3]. At the same time, it was found from calculations based on the density functional that the long-range order is preserved up to one layer. Therefore, this connection is promising for information storage devices. It should be noted that it has not yet been possible to obtain an almost single-layer structure of this compound.

The compound Fe_3GeTe_2 was first synthesized in the 2006 [1]. It crystallizes into a hexagonal structure described by a spatial group $P6_3/mmc\left(D_{6h}^4\right)$. Iron atoms occupy two nonequivalent crystallographically positions, denoted in [4] as 2*c* and 4*e* respectively. For the stoichiometric composition, provided that the positions are fully occupied, the Fe mixed valence formula for the transition metal atom can be written according to (Fe^{2+}) (Fe_2^{3+}) (Ge^{4-}) (Te_2^{2-}) [1]. The connection is layered. Each layer is a sandwich structure with two layers of tellurium atoms covering a triple layer Fe_3Geon both sides [1]. Below 230 K, spontaneous magnetization was detected, indicating ferromagnetic behavior. There is a strong magnetic anisotropy along the *c* crystal axis. Vacancies available in the position 2*c* suppress ferromagnetic ordering.

There is much debate in the literature about the nature of the long-range magnetic order. Some papers claim that this compound is a band magnet [2, 3]. In this case, according to the authors of these papers, the Stoner criterion for ferromagnetic ordering is fulfilled.

Let us now pay attention to the applicability of the Stoner criterion itself to systems with strong electronic correlations. The presence of such correlations in the compound under consideration is indicated in [3]. It can be obtained for these systems from the Hubbard Hamiltonian [5] in the approximation when the two-particle Coulomb repulsion is replaced by a single-particle interaction. However, this approximation is physically very rough. The fact is that, in order of magnitude, the density of states at the Fermi level is inversely proportional to the Fermi energy. The Fermi energy itself is equal in order of magnitude to the integral of the electron jump to another node. The Stoner criterion allows us to conclude that the Coulomb repulsion parameter at the node is equal in order of magnitude to the jump integral. Therefore, the theory of perturbations with respect to a parameter equal to the ratio of Coulomb repulsion to the leap integral is not valid due to the fact that this ratio turns out to be of the order of unity. The Stoner criterion itself is derived precisely on the basis of this perturbation theory. In addition, the Stoner criterion overestimates the stability of the ferromagnetic phase.

In other works [6, 7, 8], attention is drawn to the fact that ferromagnetism in this compound is not described only by the presence of free electrons and it is necessary to take into account the contribution of localized electrons, as well as the presence of strong electronic correlations. It is also suggested that magnetic properties can be described in the Heisenberg model of localized magnetic moments [9, 10].

To complete the picture, we note that the bulk Fe_3GeTe_2 compound demonstrates a large anomalous Hall effect [11], the physics of the kondo lattice [12], a strong increase in the mass of the electron [13] and the magnetocaloric effect.

The purpose of this work was to analyze the magnetic phase transition from the paramagnetic phase to the ferromagnetic phase based on the renormalization group approach. At the same time, within the framework of group-theoretic consideration, an irreducible representation of a spatial group is found, along which a transition occurs, and an action is constructed that is invariant with respect to this representation. The effect of vacancies in iron positions on this transition is described under the assumption that they can be considered, based on the replica method, by analogy with frozen impurities. Within the framework of the $t-J$ model, stability of the ferromagnetic phase is analyzed, taking into account the strong electronic correlations, the presence of which was mentioned above in this compound.

2. SENTATION $P6_3/mmc(D_{6h}^4)$

It has already been said in the Introduction that the compound Fe_3GeTe_2 has a phase transition from a paramagnetic to a ferromagnetic phase with a strong c-axial anisotropy below 230 K. The magnetically ordered phase is suppressed with increasing vacancy concentration. In this case, vacancies are observed only in the position of $2c$ iron atoms. Let's analyze this transition based on the theory of phase transitions of the second kind. The results of elastic neutron scattering shown in [6] in Fig. 1 indicate that this transition belongs to the second kind.

First of all, let's find an irreducible representation (IR) of a spatial group $P6_3/mmc(D_{6h}^4)$ along which this transition can occur. In this approach, we believe that $2c(3d^6)$ and $4e(3d^5)$ magnetic moments are localized on iron ions located in crystallographic positions [4]. This representation should be part of the magnetic representation of the spatial group. Therefore, we need to first determine the nature of the magnetic representation. Let's find the last ones.

Using equality [14]

$$g\mathbf{r}_j = \mathbf{r}_i + \mathbf{a}_p, \tag{1}$$

where g is the element of the spatial group, $\mathbf{r}_j$ is the initial position of the iron ion in the zero cell $\mathbf{r}_i$ is its final position in this cell, $\mathbf{a}_p$ is the returning translation by which the atom returns to the zero cell, let's define those elements of the spatial group that leave the iron atoms in place. Let's first consider the iron ions in the position $2c$. At this position in the zero cell, the coordinates of the atoms are [15] $(2/3, 4/3, 1/2$ and $\left(4/3, 2/3, 3/2\right)$. They are set in a hexagonal coordinate system. The setting

in [15] coincides with the setting in the international tables [4].

Using equality (1), it is simple to show that atoms 1 and 2 do not change their positions (up to the returning translations) under the influence of the following elements of the spatial group (in the notation of the monograph [15]):

$$e, h_3, h_5, h_8, h_{10}, h_{12}, h_{14}, h_{16}, h_{18}, h_{19}, h_{21}, h_{23},$$

where only the "rotational" part of the element of the spatial group is indicated $g_i = \{h_i \mid \tau_i\}$, τ_i — non trivial translation. The atoms are swapped by the action of the remaining elements of the group. For the position, the 4*e* iron atoms do not change their position under the action of the elements $e, h_3, h_5, h_{19}, h_{21}, h_{23}$. Now let's find the characters of the elements of the magnetic representation, which for the zero wave vector are determined by the equalities [14]

$$\chi_m^{\mathbf{k}=\mathbf{0}} = \mathrm{Sp}\, R_h \delta_h \sum_j \delta_{j,gj}, \tag{2}$$

where $\chi_m^{\mathbf{k}=\mathbf{0}}$ is the character of the element of the group, Sp R_h is the sum of the diagonal elements of the rotational part of the element g, $\delta_h = 1$ for elements of the first kind [16] and $\delta_h = -1$ for elements of the second kind, the delta symbol $\delta_{j,gj}$ means that the summation goes over those atoms that do not move under the action of the element g. From equality (2) we obtain the following values of non-zero character elements in the magnetic representation

$$\begin{gathered}\chi_m^{\mathbf{k}=0}(e) = 18,\\ \chi_m^{\mathbf{k}=0}(g_8) = \chi_m^{\mathbf{k}=0}(g_{10}) =\\ = \chi_m^{\mathbf{k}=0}(g_{12}) = \chi_m^{\mathbf{k}=0}(g_{16}) = -2,\\ \chi_m^{\mathbf{k}=0}(g_{19}) = \chi_m^{\mathbf{k}=0}(g_{21}) = \chi_m^{\mathbf{k}=0}(g_{23}) = -6,\\ \chi_m^{\mathbf{k}=0}(g_{14}) = \chi_m^{\mathbf{k}=0}(g_{18}) = 4.\end{gathered} \tag{3}$$

The characters of the other elements of the group are zero. In the usual way, using the data of the monograph [15] concerning the IR group $P6_3/mmc(D_{6h}^4)$, we find that the magnetic representation includes only two two-fold one-dimensional representations of this group, namely, $2\tau_3$ and $2\tau_6$.

Let us now consider the values [14]

$$\begin{gathered}\mathbf{S}_\lambda^{\mathbf{k},\zeta}(i) = \sum_{h \in G_k^0} d_{\lambda[\mu]}^{*\mathbf{k}\zeta} \delta_{i,gj} \delta_h \times\\ \times \exp(-i\mathbf{k} \cdot \mathbf{a}_p(g,j)) \times \left(R_{x,[\beta]}^h, R_{y,[\beta]}^h, R_{z,[\beta]}^h\right),\end{gathered} \tag{4}$$

which can be interpreted as vectors of atomic magnetic moments of the system forming a magnetic structure with a wave vector $\mathbf{k}$. In equality (4), the $d_{\lambda[\mu]}^{*\mathbf{k}\zeta}$ is conjugate matrix element of the ζ -th IR of the spatial group, the indices μ, j, β must be fixed, G_k^0 is the point group of the wave vector. Note that for ferromagnetic ordering, the wave vector is zero.

It can be shown, based on equality (4), that the representation τ_3 allows the existence of only a vector $\mathbf{S} = (0,0,1)$ on iron ions in position 2*c*, i.e., their magnetic moments are oriented along the axis z. Since all the elements of the spatial group are even elements for magnetization [17], the spatial inversion g_{13} in the notation of the monograph [15] does not change the direction of the magnetic moment $\{h_{13} \mid 000\} M_z = \delta_{h_{13}} (-M_z) = M_z$. Similarly, it is established that for the position of 4*e* iron ions, the representation τ_3. Thus, the theory of groups allows the transition to a ferromagnetic state with anisotropy along the axis z only in IR τ_3 .

Let us now note that the decomposition of the magnetic representation according to the IR of the spatial group, taking into account two-dimensional representations, includes two-dimensional representations $2\tau_9, 2\tau_{12}, \tau_{10}, \tau_{11}$. These representations, however, do not generate vectors $\mathbf{S}$, oriented along the axis z.

Thus, we conclude that the transition from the paramagnetic state to the ferromagnetic phase can only occur according to the representation τ_3 , and iron atoms in both crystallographic positions participate in the formation of the long-range order. Note that the group-theoretic analysis confirms that this phase will have anisotropy along the axis z.

Let 's return now to the presentation τ_3. The phase transition from the paramagnetic to the ferromagnetic phase is characterized by a one-component order parameter, which is denoted as $\varphi(x)$. Then the action S, invariant with respect to the representation τ_3, is written as

$$S(\varphi) = \int d^d x \left(\begin{array}{c} -\frac{1}{2}\frac{\partial\varphi(x)}{\partial x}\frac{\partial\varphi(x)}{\partial x} - \\ -\frac{\xi}{2}\varphi^2(x) - \frac{b}{24}\varphi^4(x) \end{array} \right), \quad (5)$$

where $\xi = T - T_C$, T is the temperature of the system, T_C is the Curie seed temperature, b — is the charge [18] (a constant characterizing the interaction in the system). Expression (5) completely coincides with the non-normalized action of the one-dimensional model φ^4. The description of the phase transition based on this model by the renormalization group method is well known [19, 20]. A stable critical point is found and all critical indices in the 5-loop approximation are determined. We will not write them out here. They can be found, for example, in the monograph [18].

The effect of vacancies on this phase transition will be carried out similarly to the accounting of frozen impurities in the replica method. Then the accounting of vacancies can be carried out in the form of an addition to the usual φ^4 interaction action of the form [21]

$$V_{vac} = \int d^d x \psi(x)\varphi^2(x), \quad (6)$$

where $\psi(x)$ is a Gaussian random field of vacancies with an average value

$$\langle\psi(x)\rangle = 0$$

and a correlator

$$\Delta_\psi(x) = \langle\psi(x)\psi(x')\rangle = \lambda_0\delta(x - x')$$

with a primeval constant $\lambda_0 > 0$, proportional to the vacancy concentration, $d = 4 - 2\varepsilon$, $\varepsilon \ll 1$, d is the dimension of the space. The formal description of vacancies by the replica method allows you to apply n-component field φ_a, $a = 1,\ldots,n$ n with a non-normalized action

$$S_1 = \int d^d x \left\{ \begin{array}{c} -\frac{\psi^2(x)}{2\lambda_0} - \frac{1}{2}\frac{\partial\varphi_a(x)}{\partial x}\frac{\partial\varphi_a(x)}{\partial x} - \\ -\frac{\xi}{2}\varphi_a(x)\varphi_a(x) - \frac{b}{24}\sum_a\varphi_a^4(x) + \\ +\psi(x)\varphi_a(x)\varphi_a(x) \end{array} \right\}. \quad (7)$$

Equality (7) implies summation by repeating indexes. Since we are not interested in the properties of the vacancies themselves, in action (7) we can get rid of the field $\psi(x)$. Let's integrate the functionality for this

$$Z = \int D\psi\, D\varphi \exp\left\{ \int d^d x \left(\begin{array}{c} -\frac{1}{2}\frac{\partial\varphi_a(x)}{\partial x}\frac{\partial\varphi_a(x)}{\partial x} - \\ -\frac{\xi}{2}\varphi_a(x)\varphi_a(x) - \frac{b}{24}\sum_a\varphi_a^4(x) \end{array} \right) \right\} \times \quad (8)$$
$$\times \exp\left\{ \int d^d x \left(-\frac{\psi^2(x)}{2\lambda_0} + \psi(x)\varphi_a(x)\varphi_a(x) \right) \right\},$$

where

$$D\varphi = \prod_a D\varphi_a,$$

a meaningful statistical sum, by field $\psi(x)$. This can be done precisely, since the functional integral over this field is Gaussian. We have

$$\int D\psi \exp\left\{ \int d^d x \left(-\frac{\psi^2(x)}{2\lambda_0} + \psi(x)\varphi_a(x)\varphi_a(x) \right) \right\} = \quad (9)$$
$$= \exp\left\{ \int d^d x \frac{\lambda_0}{2}(\varphi_a(x)\varphi_a(x))^2 \right\} \sqrt{2\pi\lambda_0}.$$

Then action (7) can be rewritten as

$$S_1 = \int d^d x \left\{ \begin{array}{c} -\frac{1}{2}\frac{\partial\varphi_a(x)}{\partial x}\frac{\partial\varphi_a(x)}{\partial x} - \\ -\frac{\xi}{2}\varphi_a(x)\varphi_a(x) - \frac{b}{24}\sum_a\varphi_a^4(x) - \\ -\frac{b_1}{24}\left(\varphi_a(x)\varphi_a(x)\right)^2 \end{array} \right\}, \quad (10)$$

where $b_1 = -12\lambda_0$, and $\sqrt{2\pi\lambda_0}$ we omitted as insignificant. Action (10) is an action for a dual-charge-model $O_n\varphi^4$. A complete analysis of the critical behavior of such a model in the two-loop approximation is given in the monograph [18]. The peculiarity of the case under consideration is that at the end of the calculations it is necessary to put $n = 0$ [18].

It turns out that in this case it is necessary to build decompositions not by a small parameter ε, but by

$\sqrt{\varepsilon}$ [22]. For this situation, $n = 0$ critical indices are found in the three-loop approximation (in the limit) [23]. The behavior of magnetization M in the vicinity of the critical point, based on the data [23], has the form

$$M \sim \mid T - T_c^* \mid^{\beta},$$

$$\beta = \frac{1}{2} - \frac{3}{4}\left(\frac{6}{53}\right)^2 \sqrt{2\varepsilon} - \frac{1284 + 189\zeta(3)}{53^2}\varepsilon,$$

T_c^* — the temperature of transition to the ferromagnetic phase, ζ is the Riemann zeta function. However, for the model under consideration, the stability of the critical point may be violated if the inequality holds

$$-12\lambda_0 + b < 0 \qquad (11)$$

As the vacancy concentration increases, the positive constant λ_0 increases in magnitude, which will lead to the fulfillment of (11). Then the transition to the ferromagnetic phase will be suppressed.

The approach used above, based on group-theoretic analysis, was based on the assumption that the magnetic moment is localized on iron ions. The rationale for its presence within the framework of the zone theory is as follows. It has long been known in the band theory of metals that the wave functions of d states are very strongly localized inside the atomic backbone. Therefore, their overlap between neighboring atoms can lead to the formation of only narrow zones. In transition metals, not all internal d levels are filled and they are close to s- the p-levels of valency electron. Hybridization of s- and p-levels leads to the emergence of a conductivity zone. The narrow d zone is located inside the conduction band and hybridizes with it at the points where these zones intersect [24]. This hybridization leads to the fact that the d electrons are only partially localized. The fact is that when a crystal is formed, the atomic wave functions of electrons disappear due to the overlap of atomic potentials. However, this disappearance will not always be complete; for example, virtual connected states may persist near the initial d-levels. The wave function in these states is characterized by a large amplitude inside the core, but is not strictly localized there [24]. As a result, the electron is most likely located on the transition ion, participating in the formation of a local moment, but there is a possibility that it is also involved in conduction. However, this one-electron approach to substantiate the appearance of a local magnetic moment in highly correlated $3d$ transition metal-based metals does not work well. The approach using the Hubbard model turns out to be more appropriate. For the strong repulsion of two electrons at a node, two Hubbard subzones of once and twice occupied states appear in the electronic spectrum of this model [25]. If the repulsion at the node tends to infinity, and the average number of electrons at the node is less than one, then the number of pairs tends to zero. Then the once occupied states form local magnetic moments [25].

Therefore, let us approach the problem of the appearance of a ferromagnetic phase in a compound Fe_3GeTe_2 using the Hubbard model, or rather $t - J$ model. The only condition that we need from the previous consideration is that the transition takes place according to a one-dimensional representation. Therefore, we assume that the Hubbard model for non-degenerate electrons can be used to describe the ferromagnetic state. Let's explain what is meant by the words non-degenerate electrons in this model. It is known [24] that the general model of interacting electrons, the band structure of which can be described in the strong coupling approach, is extremely difficult to study. A significant simplification for studying the properties of such electrons is carried out in the Hubbard model, in which only one orbitally non-degenerate level is essential for research, and all other levels are not included in the consideration. The latter statement is based on the assumption of a large energy gap between these levels and the selected level.

In [6], the value of the parameter U, describing the Coulomb repulsion of electrons at one node $U \approx 5$ eV is given. With such a large value of the parameter, the U term in the Hubbard Hamiltonian describing the Coulomb repulsion of electrons at a node is considered as the Hamiltonian of the zero approximation, and the kinetic term associated with the jump of an electron to a neighboring node plays the role of a perturbation [5]. Excluding from consideration the state of a system with two electrons at a node and discarding terms that depend on three nodes, one can find a Hamiltonian of the t–J model in which the Hamiltonian of the zero approximation is linear with respect to Hubbard operators, and the

perturbation is quadratic with respect to these operators. The latter circumstance makes it possible to construct a diagrammatic technique for Hubbard operators, in which the electronic Green function and the Green functions for transverse and longitudinal spin components differ significantly from those in the diagrammatic technique for fermionic and spin operators [5].

The Hamiltonian of the t–J model has the form

$$H = t\sum_{i,j,\sigma} X_i^{\sigma 0} X_j^{0\sigma} + \\ +J\sum_{i,j}\left(X_i^{-+}X_j^{+-} - X_i^{++}X_j^{--}\right). \quad (12)$$

In the Hamiltonian (12) t — the matrix element of the electron jump to a neighboring node, $X_i^{\alpha\beta}$ — the Hubbard operatorα, $\alpha,\beta = 0,+,-$, where «+» means a state with spin up, «–» — a state with spin down, «0» — a state without spin at the node, J — the exchange integral. For this model, it was shown in [5] that the Fourier image of the Green function for transverse spin components,

$$D_\perp(1-2) = \left\langle T\,\widetilde{X}^{+-}(1)\,\widetilde{X}^{-+}(2)\right\rangle, \quad (13)$$

where T is the time ordering, the symbol "tilde" means the representation of the interaction in the paramagnetic state in a generalized approximation of random phases can be written as

$$-D_\perp^*(k) = \chi(k) = \chi_0(k)\begin{pmatrix}\left[1-\Lambda(k)\right]\left[1-Q(k)\right]+\\ +\chi_0(k)\left[\Phi(k)+J(k)\right]\end{pmatrix}^{-1}. \quad (14)$$

In the last equality

$$\chi_0(k) = \frac{1}{2}\frac{n_0}{T}\delta_{\omega(n),0} - \Pi(k),$$

$\omega(n)$ — Matsubara frequency,

$$n_0 = 2\exp\left(\frac{\mu}{T}\right)\left(1+2\exp\left(\frac{\mu}{T}\right)\right)^{-1},$$

and the values Λ, Q, Π, Φ in the paramagnetic phase are determined by the equalities

$$\Pi(k) = \frac{1}{N}\sum_{k(1)} G\left(k(1)-k\right)G(k(1)\Big),$$

$$Q(k) = \frac{1}{N}\sum_{k(1)}\varepsilon\left(k(1)\right)G(k(1)-k)\,G(k(1)\Big),$$

$$\Lambda(k) = \frac{1}{N}\sum_{k(1)}\varepsilon\left(k(1)-k\right)G\left(k(1)-k\right)G\left(k(1)\right), \quad (15)$$

$$\Phi(k) = \frac{1}{N}\sum_{k(1)}\varepsilon\left(k(1)-k\right)\varepsilon\left(k(1)\right)\times \\ \times G\left(k(1)-k\right)G\left(k(1)\right),$$

where N is the number of lattice nodes. In the latter relations, the electronic Green function is taken as

$$G(k) = \left(i\omega(n) - E(\mathbf{k})\right)^{-1}, \\ E(\mathbf{k}) = \left(1-\frac{n}{2}\right)\varepsilon(\mathbf{k}) - \mu, \quad (16)$$

where n is the average number of electrons at a given node, μ is a chemical potential.

After the analytical continuation

$$i\omega(n) \to \omega + i\delta$$

expression (14) describes the susceptibility of the paramagnetic phase. In the monograph [5], a statement is formulated that ($\chi_0(\mathbf{k},\omega)$ represents the sum of contributions from localized and collectivized states of electrons. The localized contribution, inversely proportional to temperature, corresponds to Curie's law. The collectivized contribution is Paulian. This contribution associated with the electron loop is responsible for the susceptibility of the gas of non-interacting free electrons. In the same monograph, it is shown that at Fermi energy, the $\varepsilon_F > 0$ paramagnetic phase loses stability at $T = 0$, as can be seen from (14) if the condition is fulfilled

$$\Phi(0,0) + \kappa tz < 0, \quad (17)$$

that is,

$$\kappa tz < \frac{\varepsilon_F^2}{(1-n/2)^2}N\left(\frac{\varepsilon_F}{1-n/2}\right). \quad (18)$$

In inequality (17) $\kappa = t/U$, z is the number of nearest neighbors, $N(\varepsilon)$ the density of states of the initial electronic zone before its splitting into two Hubbard subzones [5]. It can be seen that at $k = 0$ ($U \to \infty$) the ground state is ferromagnetic at zero

temperature. With growth of κ ferromagnetic state is suppressed. Thus, it follows from the t -J model that both localized and free electrons participate in the formation of the ferromagnetic phase.

CONCLUSION

The paper analyzes the magnetic phase transition of the second kind from the paramagnetic to the ferromagnetic phase in a layered van-der Waals compound Fe_3GeTe_2. An important component of this consideration was to establish the fact that magnetic moments localized on iron atoms participate in the formation of a long-range magnetic order. This was done within the framework of the group-theoretic definition of the irreducible representation of the spatial group $P6_3/mmc(D_{6h}^4)$, through which the transition takes place, based on the initial assumption of the presence of such magnetic moments. It is shown that the magnetic transition into a uniaxial ferromagnetic with a moment orientation along the axis of the c crystal can occur only according to the representation τ_3, the basic function of which is the magnetic moment with the above orientation. It is important to pay attention to the fact that the group-theoretic analysis implicitly takes into account all the interactions responsible for the formation of both the crystal structure and the magnetic state of the system. The transition order parameter turns out to be one-dimensional. An action of the system is constructed that is invariant with respect to the representation τ_3. This action coincides with the action of the one-dimensional φ^4-model. Therefore, all critical indices of this transition are known, obtained from renormalization group analysis.

The influence of vacancies on this transition was carried out using the replica method and reduced to the description of a two-charge $O_n\varphi^4$ model in the limit $n \to 0$ in the final results. The renormalization group analysis of the problem in this limit was carried out in the works mentioned above. Based on these results, the temperature behavior of the magnetic moment near the critical point is found, and a condition is given under which ferromagnetism is suppressed by vacancies.

Calculations carried out in [6] based on the Hubbard model showed that for the studied compound, the electron repulsion parameter at the $U \approx 5$ eV node. Based on this result, it was assumed that the stability of the ferromagnetic phase can be analyzed using the t–J - model for non-degenerate electrons. In this case, it is possible to show that both localized and free electrons participate in the formation of ferromagnetic ordering. Free electrons provide a Paulian contribution to the dynamic magnetic susceptibility of the system.

Thus, the Stoner criterion, which is an indication that the long-range magnetic order is formed only by free electrons, is not accurate in the Fe_3GeTe_2.

FUNDING

The work was performed within the framework of the state assignment Quantum code, Grant 122021000038-7.

REFERENCES

1. H. -J. Deiseroth, K. Aleksandrov, C. Reiner et al., Eur. J. Inorg.Chem. 2006 (8), 1561 (2006).
2. H. L. Zhuang, P. R.C. Kent, Phys.Rev.B 93, 134407 (2016).
3. A. F. May, S. Calder, C. Cantoni et al., Phys. Rev.B 93, 014411 (2016).
4. International Tables for Crystallography, Vol.A. Space Group Symmetry, ed. by T. Hahn, Springer (2002).
5. Yu.A. Izjumov, M. I. Katsnelson, Yu. N. Skrjabin. Magnetism of itinerant electrons, Fizmatlit, Moscow (1994) (in Russian)
6. X. Bai and F. Lecherman, Phys.Rev.B 106, L180409 (2022).
7. X. Xu, Y. W. Li, S. R. Duan et al., Phys.Rev.B 101, 201104 (R) (2020).
8. J. -X. Zhu, N. Janoschek, D. S. Chaves et al., Phys. Rev.B 93, 144404 (2016).
9. Y. Deng, Y. Yu, Y. Song et al., Nature (London) 563, 94 (2018).
10. Y. Zhang, H. Lu, X. Zhy et al., Sci.Adv., 4, eaao6791 (2018).
11. K. Kim, J. Seo, E. Lee et al., Nat.Mater. 17, 794 (2018).
12. M. Zhao, B. -B. Chen, Y. Xi et al., Nano Lett. 21 \, 6117 (2021).
13. B. Chen, J. Yang, H. Wang et al., J.Phys. Soc. Jpn. 82, 124711 (2013).
14. Yu.A. Izjumov, V. E. Naish, R. P. Ozerov, Neutronography of magnets, Atomizdat, Moscow,(1981) (in Russian)

15. O.V. Kovalev, Irreducible and induced representations and co-representations of Fedorov groups, Nauka, Moscow (1986) (in Russian)

16. Yu.I. Sirotin, M. P. Shaskolskaya, Fundamentals of crystal physics, Nauka, Moscow (1979). (in Russian)

17. V.V. Men'shenin, FMM 115, 1057 (2014).

18. A.N. Vasiliev, Quantum field renormalization group in the theory of critical behavior and stochastic dynamics, Publishing House PNPI, St. Petersburg (1998) (in Russian)

19. K.G. Wilson and M. Fisher, Phys.Rev. Lett. 28 240 (1972).

20. Sh. Ma, Modern theory of critical phenomena, W.A. Benjamin. Inc. (1976)

21. A.B. Harris and T.C. Lubensky, Phys.Rev. Lett. 33, 1540 (1974).

22. D.E. Khmelnitsky. JETP. 68, 1960 (1975).

23. B.N. Shalaev, JETP 73, 2301 (1977).

24. J.M. Ziman, Principles of the Theory of Solids, Mir, Moscow (1974).

25. V.Yu. Irkhin, Yu. P. Irkhin, Electronic structure, physical properties and correlation effects in d- and f-metals and their compounds, Ekaterinburg (2004)