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4f-local magnetic moments in the metals and alloys with SDW-instability

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Résumé. — L'hamiltonien considéré dans cet article décrit les interactions entre les moments magnétiques localisés et les électrons de conduction (terme RKKY), ainsi que le couplage entre les électrons et les trous de la surface de Fermi possédant un terme de « nesting ». La présence d'impuretés ayant un moment magnétique localisé conduit à l'apparition d'ondes de densité de spin pour les électrons de conduction. Ceci reste vrai même dans le cas où le terme de « nesting » et la constante de couplage triplet entre électrons et trous sont très petits. Le calcul du diagramme des phases magnétiques a été fait en tenant compte de la diffusion des électrons par les fluctuations des spins localisés. L'influence du champ magnétique extérieur sur la température de Néel et la structure magnétique a été étudiée. Nous espérons que des expériences de diffraction de neutrons sous champ magnétique pourront confirmer notre proposition.

Abstract. — The usual interaction between localized magnetic moments and itinerant electrons (RKKY-coupling) is modified by the additional coupling between nesting electrons and hole parts of the Fermi surface. It is shown that the presence of localized magnetic moments of magnetic impurities leads to the appearance of spin-density-waves in the itinerant electron system even in the case where nesting is bad and the constant of triplet electron-electron interaction is small. In order to calculate the magnetic phase diagram we also introduce the effect of the scattering of the itinerant electrons on the localized spin fluctuations. In addition the influence of external magnetic field on the Néel temperature and magnetic structure is discussed and new experiments are proposed.

1. Introduction.

There is much current interest in the metallic materials which contain either 4f-local magnetic moments or itinerant d-electrons. The coupling between both systems is described usually by using the RKKY-interaction but standard theory neglects the coupling between itinerant electrons, which leads to the magnetic instability according to the Stoner-like theory.

This paper is devoted to metallic antiferromagnets (AF) with incommensurate spin structures. The helical AF order for local spins in rare earth metals was discussed for the first time by Dzyaloshinsky [1] which pointed out that the Fermi surface topology for the itinerant electrons determines the type of magnetic order and AF structure wave vector \( Q \) for the local spins (see also the articles by Vul' and Krivoglaz [4, 5]). It is also well-known that the instability in the itinerant electron system against the appearance of the spin-density-wave (SDW) occurs in the metals with nesting-type Fermi surface. For this topology the exchange by triplet electron-hole pairs leads to the appearance of antiferromagnetic order, with vector \( Q \) equal to the nesting vector of the Fermi surface.

Incommensurate SDW in the AF chromium is a clear example for such instability. Therefore the problem concerning the behaviour of the local magnetic moments in the system with SDW-instability emerged at first time during the discussion for the properties of chromium — rare earth metal dilute alloys [2, 3]. In the framework of the excitonic insulator model (in the mean field approximation) the influence of local spins was considered by Volkov and Mnatsakanov [6] and by Ami and Young [7]. These papers are however restricted to the case of commensurate SDW in the limit of the small contents of rare earth impurities.
In our previous paper [8] such type of approach was used for the description of the incommensurate helical antiferromagnetism in yttrium-heavy rare-earth-metal (HREM) alloys. The magnetic phase diagrams $T(x)$ were calculated in the range $(0 < x < 1)$ of the alloy composition $Y_{1-x}R_x$ ($x$ is the concentration of HREM's in the alloy).

The physical picture of the antiferromagnetic ordering is now discussed. The appearance of the local magnetic moments in the itinerant electronic system with the nesting of electrons and holes at the Fermi surface initiates the rise of SDW ordering. It occurs even for a system with a small value of the coupling constant for the triplet interaction between electrons and holes and also when bad nesting do not provide the SDW rise in the pure metal. The local spins are the source of the order parameter in the self-consistency equation. Simultaneously the SDW are related to the local moments at the impurity sites leading to correspondence with the magnitude of the SDW exchange field at these states.

It is well-known that the transition temperature $T_N$ for the system with SDW instability is sensitive to the scattering on impurities and phonons. In the case of Y-HREM alloys the main contribution to the scattering effects is the scattering of SDW on the local moment fluctuations. This is a consequence of the isoelectronic character of HREM impurities for which the scattering on the charge fluctuations is negligible.

The influence of the scattering effects on the antiferromagnetic ordering for such systems has not being examined. It is interesting to investigate whether the spin fluctuations decrease the Néel temperature $T_N$. In section 2, we describe the experimental situation and the results of band structure calculations for yttrium-HREM's and Eu. Section 3 presents the model and explains the method of calculation together with the results obtained. The influence of the homogeneous external magnetic field on the transition temperature is discussed in section 4. In section 5 some conclusions are drawn.

2. Electronic and magnetic structures for hexagonal alloys of the yttrium with HREM and for cubic europium

The experimental situation in the alloy $Y_{1-x}R_x$ is reported in the book of Coqblin [9]. In the yttrium-HREM (Tb, Dy, Ho, Er, Tm) alloys the antiferromagnetic transition takes place at every concentration $x$, except for the small concentration region $(x < 0.05)$ where the situation is not clear. However, the helical magnetic structure with incommensurate wave vector $Q$ which is parallel to hexagonal axis $X$ is present only for the alloys with Tb, Dy and Ho (and also with Gd), whereas the alloys with Er and Tm have the sine-shaped SDW with the $Q$ vector along the same axis. At temperature $T_c < T_N$ all concentrated alloys $Y_{1-x}R_x$ with the helical SDW present a transition into the ferromagnetic phase whereas, for the sine-shaped alloys such transition was not found. The structure of the ferromagnetic phase for all alloys coincides with the magnetic structure of the pure HREM.

It should be noted that the angle of helix $\omega = \frac{1}{2}QC$ ($C$ is the lattice parameter) depends on the concentration $x$ and temperature. It is interesting to note that although pure yttrium is a paramagnet at all temperatures, dilute alloys $Y_{1-x}R_x$ present the helical antiferromagnetic structure (even for small concentration $x \approx 0.05$) with angle of helix $\omega = 50^\circ$ close to the angle in the helical phase of pure HREM's at Néel temperatures.

The band structure of yttrium is similar to that of HREM's which has the same HCP crystal lattice. From band structure calculations (see for example [10, 11]) it is known that the paramagnetic Fermi surface of yttrium, like HREM's have the nesting electron and hole parts along the LH lines of Brillouin zone. It means that these nesting parts of the electronic bands can be approximately expressed by the following form:

$$\begin{align*}
\epsilon_1(k) &= \xi (k_z) + \mu_1(k_\perp) \\
\epsilon_2(k + \vec{Q}) &= -\xi (k_z) + \mu_2(k_\perp)
\end{align*}$$

where $\xi (k_z) = V_{f} K_{z}$, $\vec{Q}$ is the geometrical nesting vector for electron and hole parts, $\mu_{1,2}(k)$ characterizes the nesting imperfection. The $z$ axis is parallel to hexagonal $C$ axis ($T$A line in the Brillouin zone) and $k_\perp$ vector is parallel to the LH line. We will omit the band indices from now on.

The reason of the lack of SDW in the pure yttrium connects with bad nesting (large value of $\mu (k_\perp)$) and the small value of the triplet coupling constant $g_{\nu}$. However the band structure calculations [11] show that the magnitude of $\vec{Q}$ vector for pure yttrium coincides with the magnitude of $Q$ wave vector for the helical AF structure in the yttrium alloys. It should be emphasized once more that the HREM's, except Gd, have a Fermi surface similar to the nesting electron and hole parts described by equation (1). Thus, the appearance of SDW in the yttrium alloys and in the pure heavy rare-earth metals is explained by the existence of the nesting at the Fermi surface and by the presence of 4f-local magnetic moments in the system.

At the same time the europium metal which possesses only two (not three) electrons in the valence bands and another type (bcc) of crystal lattice has a completely different Fermi surface topology together with the helical incommensurate AF structure of wave vector $Q = 0.29 2 \pi/a$. Indeed, the band structure calculations [12-14] have demonstrated the presence of the nesting parts at the Fermi surface in the europium case too. Moreover the calculated nesting vector $Q = 0.33$ (in units $2 \pi/a$) agree with the experimental value of $Q$. 


(both vectors are parallel to one of cubic axes (100)-type). It means that the general form for the nesting-type spectrum (Eq. (1)) can be also used for the description of the antiferromagnetic ordering in europium.

3. Method of calculation and results.

The starting point of this approach can be described by the following model Hamiltonian:

\[ H = H_{bs} + H_{ce} + H_{cs} \]  
(2)

where \( H_{bs} \) represents an itinerant electron system, and \( H_{ce} \) corresponds to the coupling between itinerant electrons (density-density interaction) with different moments and band indices. \( H_{bs} \) and \( H_{ce} \) are written as follows:

\[ H_{bs} = \sum_{k,\sigma} \varepsilon(k) a_{k\sigma}^{+} a_{k\sigma}; \]

\[ \varepsilon(k) = -\varepsilon(k + Q) \]  
(3a)

and:

\[ H_{ce} = \sum_{k,k',\sigma,\sigma'} g(k, k', q) a_{k\sigma}^{+} a_{k'\sigma'} a_{k'q\sigma'} a_{k+q\sigma} \]  
(3b)

where \( a_{k\sigma}^{+} \) and \( a_{k\sigma} \) are creation and annihilation operators for the itinerant electrons, \( \sigma \) and \( \sigma' \) are spin indices.

The third term in Hamiltonian (2) is:

\[ H_{cs} = -\sum_{n,k',\sigma} J_a(k, k') \times N_x(n) \sum_{\sigma} a_{k\sigma}^{+} a_{k'\sigma} \]  
(4)

where:

\[ J_a(k, k') = J(k, k') \exp\left(i(k-k')R_n\right) \]

\[ J(k, k') = \int dr \psi_k(r) J(r) \psi_k^{*}(r). \]

Here \( J(r) \) is the exchange potential of the RKKY-interaction between the localized spins \( S \) at \( R_n \)th lattice sites and the itinerant electrons. \( \hat{\sigma} \) is the Pauli matrix. \( N_x(n) = 0.1 \) is a probability to have the localized spins \( S \) at \( R_n \) for the alloys with the concentration \( x \).

The antiferromagnetic order parameter (self-consistent exchange field):

\[ \Delta_{Q}^{\sigma} = g(Q) \sum_{k} \left\langle a_{k\sigma}^{+} a_{k+Q\sigma} \right\rangle_{\sigma'\sigma'} \]  
(6)

has the following symmetry:

\[ \left( \Delta_{Q}^{\uparrow} \right)^{*} = \Delta_{Q}^{\downarrow}; \]

\[ \Delta_{Q}^{\downarrow} = \Delta_{Q}^{\uparrow} = 0 \]  
(7)

in the case of the helical AF structure, but in the case of the sine-shaped AF structure the symmetry is the following:

\[ \Delta_{Q}^{\uparrow} = \Delta_{Q}^{\downarrow} = 0, \Delta_{Q}^{-} = \Delta_{Q}^{+}. \]  
(8)

We first discuss the helical SDW case. It should be noted that in the real metals the wave vector \( Q \) of SDW does not coincide with the mean nesting vector \( \bar{Q} \). The difference occurs because the free energy minimum which determines \( Q \) is a compromise between the contributions from different parts of non-ideal nested Fermi surfaces (parameters \( \mu_1(k) \neq 0 \) [15]). For simplicity we assume that \( Q = \bar{Q} \) and then all our results are equivalent for both (helical and sine) cases. However experimental measurements [9] show the significant concentration and temperature influence on the \( Q \) vector. The concentration dependence can be explained through the concentration dependence of the one-particle spectra in equation (1), but the temperature dependence of \( Q \) has no such explanation. It means that really vectors \( Q \) and \( \bar{Q} \) are different.

In order to give a qualitative explanation of phase diagrams we assume that these vectors are equal. Moreover we assume for simplicity that \( \mu_1(k) = \mu_2(k) = \mu_0 \left( k_\perp / k_F \right) \), where \( k_F \) is an average value of the Fermi vector.

Finally, our problem is to get a solution of the self-consistent equation relating the order parameter \( \Delta \) to the mean thermodynamic value of local magnetic moment at atomic site. It should be emphasized that only nesting parts of the Fermi surface are important for the SDW formation whereas the effective frequency for the scattering on the local spin fluctuations depends on the whole Fermi surface electrons. Thus we will extent a procedure described previously [11] in order to take into account the scattering on the local spin fluctuation at the atomic site. According to our remark, the renormalization of the scattering frequency \( \tau^{-1} \) during the SDW formation below the transition temperature is related to the ratio of the density of states at the nesting parts by the whole density of states at the Fermi level; this is about 0.1.

The bare temperature Green function may be written as:

\[ \tilde{\Sigma}_{Q}^{\sigma} = \left( i\omega_n - \varepsilon(k) + i\tau^{-1} \text{sign} \left( \omega_n \right) \right)^{-1} \]  
(9)

where \( i\omega_n = \pi T (2n + 1) \). We introduce the renormalized value of the antiferromagnetic gap:

\[ \Delta_{Q}^{\sigma} = \Delta_{Q}^{\sigma} + J_{Q} \left\langle \hat{\delta}_{n} \hat{\sigma} \exp \left( \pi i Q R_n \right) \right\rangle_{\sigma' \sigma} \]  
(10)

which must be included in the Green function equation of motion.

By using the definitions (9) and (10) we find the self-consistent equation for order parameter \( \Delta_{Q}^{\sigma} \) which is similar to equation (10) of our previous paper [11]. Assuming linear approximation for the \( \Delta \) parameter (indices are omitted) in this equation, we may write:

\[ \Delta = \pi T \times U \int_{y}^{1} \sum_{y = -y_{\text{max}}}^{y_{\text{max}}} \frac{\omega_n}{\omega_n^2 + \mu_0 y^2}; \]

\[ y = k_\perp / k_F \]  
(11)
\( N_n(E_F) \) is the nesting part of the density of states, 
\( \omega_n = \omega_n \left( 1 + 1/\tau \right) \), \( \tau^{-1} \) is a scattering frequency of spins fluctuations, \( U = g_Q N_n(E_F) \). Here we used the mean field approximation for quantum average \( \langle ... \rangle_{\sigma} \) and virtual crystal approximation for the configuration average \( \langle ... \rangle \) in the second term of equation (10), i.e.:

\[
\Delta = \Delta + \frac{1}{2} J_Q \times sB_{s}(H_{\text{eff}}/T) x
\]

where \( H_{\text{eff}} = J_Q \Delta/g_Q, B_{s}(x) \) is the Brillouin function.

It is possible to calculate the phase diagram \( T_N(x) \) by using equation (11) and (12) as already performed in our previous work [11] with the assumption \( \tau^{-1} = 0 \). However, the frequency of scattering on the spin fluctuations can be obtained by the coherent potential approximation (CPA) method by using higher spin correlation functions decoupling along the lines proposed by Hasegawa [16] in the spin-fluctuation theory of itinerant magnetism, i.e. we assume:

\[
\langle S^{2k} \rangle = \langle S^{2} \rangle^k, \langle S^{2k} \pm 1 \rangle = 0
\]

where \( k = 1, 2, 3... \) Using this decoupling, from the value \( \tau^{-1} \) in the paramagnetic state, we can determine the value of the Néel temperature.

It should be noted that the potential \( J_n(Q) N_s(n) \) in the RKKY Hamiltonian (6) is a random function from the lattice position \( n \). This potential differs from zero only for these sites where the yttrium atom is replaced by an HREM atom. In the one-site approximation for CPA we find the T-matrix as:

\[
T_n = \left[ U_n - \Sigma_n(E) \right] \times \left[ 1 - F_n(E) \left( U_n - \Sigma_n(E) \right) \right]^{-1}
\]

where \( U_n = J_n(r) \cdot \left[ \frac{\delta}{\delta r} . N_s(n) \right] \) is a random value, \( \Sigma_n(E) \) is the coherent potential; the site-diagonal Green function \( F_n(E) \) is given by:

\[
F_n(E) = \langle \psi | G_n | \psi \rangle
\]

and

\[
G_n = \left( E - \varepsilon(k) + \Sigma_n(E) \right)^{-1}.
\]

The coherent potential \( \Sigma_n(E) \) is determined by the condition of CPA theory:

\[
\langle T \rangle = 0.
\]

However, in our case, this condition has an unusual form:

\[
x \langle T_n \rangle + (1 - x) \frac{- \Sigma_n(E)}{1 + \Sigma_n(E) F_n(E)} = 0
\]

and for the states with HREM atoms the T-matrix must be averaged due to the spin-fluctuation processes [16], namely:

\[
F_n(z) = \bar{F}_n(z - \Sigma(E_F))
\]

so that:

\[
F_n(z) = \bar{F}_n(z - \Sigma(E_F))
\]

where \( z \) is a complex energy.

Combining equations (18) and (16), the expression for the coherent potential becomes:

\[
2xD . U_Q^2 = \left[ 1 + \frac{4 D^2 U_Q^2}{(1 - 2 \Sigma(E_F) D)^{1/2}} \right] (19)
\]

where:

\[
D = \Sigma(E_F) + \left( \Sigma(E_F)^2 + 1 \right)^{1/2}.
\]

Results of numerical calculations (see Fig. 1) show that the imaginary part \( \Sigma(E_F) \) of the self-energy plotted as a function of the local magnetic moment concentration \( x \) is almost a linear function. It should be
Fig. 1. — Néel temperature as a function of the local magnetic moment concentration for two different cases: curve 1 represents the model without spin-fluctuation scattering, curve 2 is the \( T_N(x) \) in the model taking into account the self-energy concentration (broken line, right scale).

Also noted that the coherent potential (Eq. (19)) is the imaginary part of the self-energy. For

\[
\left| \Sigma(E_F) \right| = \tau^{-1},
\]

we have a possibility to find the solution of the gap equation (11) by taking into account the effect of the spin fluctuation scattering.

Since \( \Delta \) vanishes at \( T_N \) we can carry out an expansion of the right side of equation (12) in powers of \( \Delta \):

\[
\Delta = \Delta \left( 1 + \eta/T_N \right) \ldots
\]

where:

\[
\eta = \frac{1}{6} \frac{J^2}{g_Q}(s + 1).
\]

Substituting for \( \Delta \) in equation (11) we get, after some manipulation:

\[
\left( 1 + \eta/T_N \right)^{-1} = U\pi \left( T_N, \mu_0, \Sigma(0) \right)
\]

where the polarization operator \( \pi \) is given by:

\[
\pi \left( T_N, \mu_0, \Sigma(E_F) \right) = \ln \left( \frac{\gamma W}{\pi T_N} \right) + \phi \left( \frac{\mu_0}{\pi T_N}, \frac{\Sigma(E_F)}{\pi T_N} \right)
\]

and the function \( \phi(a, b) \) defined by:

\[
\phi(a, b) = \frac{2}{\gamma} \sum_{n=0}^{\infty} \left[ \arctan \left( \frac{a}{2n+1} + b \right) - \frac{a}{2n+1} \right],
\]

where \( \gamma \) is the Euler-Mascheroni constant.

The characteristic value of \( \mu_0 \) and the coupling parameters \( J_Q, g_Q \) or \( U \) depend on the alloy composition. In the present work in order to construct the qualitative phase diagram we expect that these model parameters are independent of the concentration \( x \). The parameters were chosen (see Table I) in order to make comparison with the experimental phase diagrams for Y-Gd and Y-Tb alloys.

We have made a rather crude approximation about the concentration independence of the band structures and wave functions of the valence electrons in Y-HREM’s alloys. The justification of this approximation is the isoelectronic character of yttrium and HREM’s, but it should be noted that the variation of the parameter \( \mu_0 \) is important because the nesting parts disappear in pure Gd.

The sole fitting parameters are the \( J_Q \) and \( U \) coupling constants determined by comparison with the experimental Néel temperature for \( x = 1 \). The value of Stoner constant \( I = g_Q \) was calculated from the real d-electron wave function at the Fermi energy and the density of states of the valence electrons of paramagnetic Y is given by self-consistent band structure calculation [11]. The calculations were made in the framework of the density functional formalism. The band width and the value of \( \mu_0 \) were also taken from the band structure calculation (Table I).

| Table I. — Parameters for the determination of the Néel temperature and of the phase diagram. \( s \) is the spin of the rare-earth, \( g_Q \) is the triplet coupling constant, \( N(E_F) \) is the density of states at the Fermi level, \( U = g_Q N(E_F) \), \( W \) is the half band-width, \( J_Q \) is the exchange potential and \( \mu_0 \) is the nesting imperfection. |
|---------------------------------|--------|-----|-----|-----|-----|-----|
| Model                          | \( s \) | \( g_Q \) | \( N(E_F) \) | \( U \) | \( W \) | \( J_Q \) | \( \mu_0 \) |
| Fig. 1                          | 7/2    | 0.022 | 28.2 | 0.025 | 0.050 | 0.0157 | 0.003 |
| Y-Tb                            | 6/2    | 0.022 | 28.2 | 0.022 | 0.050 | 0.0171 | 0.003 |

In figure 1 the results of the numerical solution of equation (21) for \( \Sigma(E_F) = 0 \) and for \( \Sigma(E_F) \) determined by equation (19) are plotted. Figure 1 shows that the scattering effect not only decreases the value of Néel temperature, but leads to more non-linear dependence of \( T_N(x) \). The comparison between the calculated and the experimental phase diagrams of Y-Tb alloys shows a satisfactory agreement even for this simplified model (see Fig. 2).

4. The influence of homogeneous magnetic field on the antiferromagnetic transition temperature.

The homogeneous external magnetic field \( H \) can change the Néel temperature \( T_N(x) \) and the form of
Fig. 2. — The magnetic phase diagram of the Y-Tb alloys. The full line represents the $T_N(x)$ dependence calculated in the present model with spin-fluctuation scattering, the circles are the experimental points from (Coqblin, 1977).

the magnetic structure. This influence is a consequence of three different reasons:

(i) At first the external magnetic field wants to align the local magnetic moments in the same direction. This effect is proportional to $\mu_B H$ for $T(x)$.

(ii) In the external magnetic field the « freezing » of spin fluctuation discussed in the preceding section occurs. This effect is proportional to $\mu_B H$ for $T(x)$.

(iii) In the external magnetic field the spin polarization of the nesting electrons which formed the SDW takes place. This effect leads to an effective change of the nesting quality proportional to $\mu_B H$ for $T(x)$.

It is obvious that effects (ii) and (iii) are negligible for the considered cases of moderate magnetic fields and of localized magnetic moments of 4f-electrons. Indeed, table I and figure 1 show that $T_N(x) \ll T^{-1}(x)$.

Let's discuss the case when the field $H$ has the direction along the helical axis. In this simplest case of sloping helix, a conical structure for which the component of magnetization along the helical axis appears, will take place. Then the Néel temperature equation (21) has the following form:

\[
\left(1 + \frac{1}{2} \times \frac{J_0^2}{gQ T_N} s B_x(\xi)\right)^{-1} = U \pi \left( T_N, \mu_0, \Sigma \left( E_F \right) \right) \tag{23}
\]

where $\xi = \mu_B H/T_N$.

For $T > T_N$ only an homogeneous component of magnetization induced by an external field exists but at temperatures below $T_N$ the SDW magnetic structure appears and the local magnetic moment slope depends on its positions in the SDW structure. Note that the magnetic moment of SDW (i.e. the itinerant electrons) does not change on direction and magnitude in the moderate magnetic fields. Thus we have the possibility to determine the magnitude of SDW magnetic moment experimentally by measuring the change of projection on the crystal plane of the magnetic moments perpendicular to the external magnetic field.

If the magnetic field has the direction of the helical plane, say along the $x$ axis, two self-consistent equations for the order parameters $\Delta_x$ and $\Delta_y$ are obtained. The axis $y$ has its direction parallel to the $c$ axis of the hcp crystal. In the limits $\Delta_x \rightarrow 0$, we find that the Néel temperature equation for the $\Delta_y$ component coincides with equation (23), but for $\Delta_x$ component we get:

\[
\left(1 + \frac{1}{2} \times \frac{J_0^2}{gQ T_N} s B_y(\xi)\right)^{-1} = U \pi \left( T_N, \mu_0, \Sigma \left( E_F \right) \right) \tag{24}
\]

Equations (23) and (24) are equivalent in the limit $\xi \rightarrow 0$.

When the temperature is decreased, the increase of $\Delta_y$ is much more rapid than that of $\Delta_x$ as it follows from equations (23) and (24). It means that the sine-shaped structure appears in the direction which is normal to the magnetic field direction. If we decrease the temperature further, the component $\Delta_x$ of the order parameter becomes important and the sine-shaped structure is replaced by the sloping helical structure. However the sine-helical transition can occur only for weak magnetic fields.

Let us consider the limiting case $\mu_B H \gg T_N(x)$ which can be realized experimentally for a small concentration $x$ in yttrium alloys. Within the same approximation equations (23) and (24) have to be replaced by:

\[
\left(1 + \frac{1}{2} \times \frac{J_0^2}{gQ T_N} x \mu_0 \frac{H}{T_N}\right)^{-1} = U \pi \left( T_N, \mu_0, \Sigma \left( E_F \right) \right) \tag{25}
\]

\[
\left(1 + \frac{1}{2} \times \frac{J_0^2}{gQ T_N} x \exp \left( -\frac{\mu_B H}{T_N} \right)\right)^{-1} = U \pi \left( T_N, \mu_0, \Sigma \left( E_F \right) \right) \tag{26}
\]

Thus we find from equations (25) and (26) that the structure with $\Delta_y \neq 0$ (Eq. (25)) appears before the structure with $\Delta_x \neq 0$ (Eq. (26)).
It is interesting to note that the Néel temperature falls with increasing magnetic field and, in principle, it can fall down to zero for some critical value of the magnetic field $H_c$:

$$
\mu_B H_c = \frac{1}{2} \frac{J^2_Q}{g_Q} \times S_x \left\{ U \left( 0, \mu_0, \Sigma \left( E_F \right) \right) \right\}^{-1} - 1 \right\}^{-1}.
$$

(27)

Therefore, the magnetic field decreases the transition temperature of AF ordering for any direction of $H$ relative to the direction of SDW vector $Q$. In the case of $H \perp Q$ it leads not only to the deformation of the AF structure but also to a possible existence of the sine-shaped AF phase. When the magnetic field increases, the value of $T_N (x)$ decreases down to zero. Thus, the phase diagram in magnetic field has the critical concentration $x_c (H)$. Below this concentration the AF order does not appear (it is known from Eq. (27) that $x_c (H) \sim H$).

5. Conclusion.

This paper is concerned with an itinerant electron system in which well-localized atomic magnetic moments exist. It was demonstrated that the appearance of these moments in the system with SDW instability leads to antiferromagnetic transition and that the wave vector of AF structure determines the nesting of the Fermi surface. The scattering on the spin fluctuations leads to a small decrease of Néel temperature, whereas the magnetic field decreases $T_N$ significantly at all orientations of $H$ and $Q$ vectors. The magnetic field can lead to a change of the helical structure on sine-structure and since the alloys with Er and Tm has the sine-shaped AF ordering without the external magnetic field it is expected that additional anisotropic interactions (omitted in our model) will make transition to sine-structure.

It should be emphasized once more that this model can be applied not only to Y-HREM alloys where $x \neq 1$ but also to pure heavy rare-earth metals and europium in which Fermi surfaces possess the nesting peculiarities. However, in the dilute solution of HREM's in yttrium, the model leads to a Néel temperature of all the concentrations of the magnetic moments ($T_N \rightarrow 0$ at $x \rightarrow 0$). It is obvious that there is a critical concentration of magnetic moments for the creation of magnetic order in the alloys, but the experiments have not being performed for $x \lesssim 0.05$.

The main conclusion of our work is that the theory of magnetic ordering in the heavy rare-earth metals and their alloys can be rewritten taking into account the electron-hole interaction in the itinerant electron system. It leads to new conclusions for the magnetic phase diagram and the values of the $T_N (x)$, as well as for the influence of the homogeneous magnetic field on the form of SDW (sine or helical).

References