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# Landau Fermi-liquid theory for heavy-fermion compounds: I. Thermodynamics

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**Abstract.** We generalize the Landau Fermi-liquid theory for describing electrons in heavy-fermion compounds. The theory gives results in good agreement with microscopic mean-field approaches. We study the low-temperature magnetic properties of the compounds and the competition between ferromagnetism and the coherent Kondo state, taking into account the RKKY interaction.

## 1. Introduction

Extensive experimental and theoretical investigations have shown that unusual low-temperature properties of heavy-fermion (HF) compounds are related to the interaction between conduction electrons and localized electrons of partially filled f shells of rare-earth or uranium ions (see, for example, the reviews in [1–7], and references therein). The partial occupancy of the f shells is caused by strong repulsion between f electrons. With decreasing temperature the interaction between conduction and f electrons plays a more and more important role, bringing about the Kondo effect and in this way forming the low-temperature properties of HF compounds. One has to distinguish two temperature regions above and below the Kondo temperature $T_K$. In the region $T > T_K$ the Kondo effect is incoherent, i.e. the Kondo screening of localized f moments takes place independently of each f ion. In that case the HF systems behave as concentrated Kondo impurity systems. To describe their properties, one can use the exact results obtained for the impurity Kondo model [6, 8, 9]. In the low-temperature region ($T < T_K$) the Kondo effect becomes coherent. As a result some properties of HF compounds differ significantly from properties of concentrated Kondo impurity systems. The coherent Kondo effect results in a strong renormalization of quasiparticle states near the Fermi surface. The corresponding quasiparticle mass is anomalously large: $m^* \simeq 10^2 m_0$. It is worth noting that, at $T \ll T_K$, HF compounds behave like normal Fermi liquids of very heavy quasiparticles and a Fermi temperature of the order of $T_K$. The interaction between conduction and f electrons has an ambivalent character. On the one hand the interaction leads to the formation of a singlet ground state owing to the Kondo effect. On the other hand it brings about the magnetic RKKY interaction between localized magnetic moments of f electrons that can stimulate long-range magnetic order. The competition between the Kondo effect and magnetism is an important feature of HF compounds and leads to a rich phase diagram [3].

At the present time the mean-field approach based on the $1/N$ expansion of large-degeneracy models is the most advanced theory for describing HF compounds [5, 10–12].

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This approach allows us to explain a number of thermodynamic and kinetic phenomena. According to the mean-field approach, at temperatures $T \ll T_K$, HF compounds behave like normal Fermi liquids in which quasiparticle states near the Fermi surface are superpositions of conduction and f-electron states. Moreover the main contribution to the wavefunctions of these states is given by f electrons. This is the reason for the large quasiparticle mass. The variational Gutzwiller approximation gives similar results [13]. Unfortunately in spite of many achievements the mean-field approach faces many significant difficulties in describing magnetism in HF compounds. Mathematical complexity is another shortcoming of the approach that makes it difficult to understand the physical peculiarities of the compounds.

We think that a generalization of the Landau Fermi-liquid theory [14, 15] for the case of electrons in HF compounds could lead to a more profound understanding of the compounds and give new opportunities for studying magnetism and kinetic phenomena. The Landau phenomenological theory has been used effectively for studying normal nonmagnetic metals (see, for example, [16]), magnetic metals [17, 18] and superconductors [19]. The phenomenological approach to electrons in the impurity Kondo model has been derived by Nozières [20] in good agreement with the exact results [8, 9]. In the present paper we develop a phenomenological Fermi-liquid approach to study electrons in HF compounds. A general formulation of our approach is given in section 2. In section 3 we apply it to investigate a paramagnetic HF. In section 4 we shall study the magnetic properties of HF systems at zero temperature. The coexistence of long-range ferromagnetic order and the coherent HF state at nonzero temperatures will be studied in section 5. Finally in section 6 we shall discuss our results.

## 2. Formulation of the phenomenological approach

At present it is generally accepted that HF compounds may be described by the lattice Anderson model with the Hamiltonian

$$H = \sum_{k\alpha} \{\varepsilon(k) c^+_{\alpha k} c_{\alpha k} + \varepsilon_f f^+_{\alpha k} f_{\alpha k} + (V c^+_{\alpha k} f_{\alpha k} + \mathrm{HC})\} + U \sum_i n_{fi\uparrow} n_{fi\downarrow}. \tag{2.1}$$

According to (2.1) the system under consideration consists of conduction electrons in the energy band $\varepsilon(k)$ with the spin $s = 1/2$ and spin index $\alpha$. There are also f electrons in a very narrow f band. If the dispersion of the f band is small enough, then f electrons may be considered as localized at lattice sites with the index $i$ on the energy level $\varepsilon_f$ under the Fermi surface, i.e. $\mu - \varepsilon_f > 0$ where $\mu$ is the chemical potential. The hybridization with the parameter $V$, which for simplicity is supposed to be independent of $k$, enables electrons to undergo a transition between conduction and f states. The unusual properties of the system are related to a large repulsion $U$ between f electrons. Owing to the repulsion the double occupancy of the f level is energetically unfavourable. In the limiting case $U \to \infty$ and $\mu - \varepsilon_f \gg \pi |V|^2 \rho_0$ where $\rho_0$ is the density of states near the Fermi surface, the lattice Anderson model is reduced to the lattice Kondo model. In that case the interaction between conduction and f electrons at the site $i$ is equal to $H_{int} = -J S_{fi} \cdot S_{ci}$, where $S_{fi}$ and $S_{ci}$ are the spins of conduction and f electrons, respectively. The local exchange interaction is antiferromagnetic, since the Kondo coupling $J = 2|V|^2/(\varepsilon_f - \mu)$ is negative. In the limiting case the occupancy $N_f$ of the f level is close to 1 and almost temperature independent.

Our phenomenological Fermi-liquid approach to electrons in HF compounds is based on two assumptions. The former is related to the ground-state structure. That is we suppose that at $T \ll T_K$ the wavefunctions of a quasiparticle with the wavenumber $k$ and spin index

$\alpha$ near the Fermi surface is a superposition of Bloch wavefunctions of electron states in the conduction band and narrow f band:

$$\Psi_\alpha(k) = A_{\alpha k}\Psi^c_\alpha(k) + B_{\alpha k}\Psi^f_\alpha(k). \tag{2.2}$$

Secondly we suppose that the number of electrons in the narrow f band is fixed. For that purpose we introduce an additional chemical potential $\lambda$.

Let us introduce a distribution function of electrons. As the system consists of conduction and f electrons we introduce two functions $N^c_{\alpha\beta}(k)$ and $N^f_{\alpha\beta}(k)$ which describes a distribution of electrons over states in the conduction and f bands. In terms of a microscopic theory these functions may be defined as

$$N^c_{\alpha\beta}(k) = \langle c^+_{\beta k}c_{\alpha k}\rangle \qquad N^f_{\alpha\beta}(k) = \langle f^+_{\beta k}f_{\alpha k}\rangle. \tag{2.3a}$$

Assumption (2.2) demands an introduction of non-diagonal components of the distribution function

$$N^{fc}_{\alpha\beta}(k) = \langle c^+_{\beta k}f_{\alpha k}\rangle \qquad N^{cf}_{\alpha\beta}(k) = \langle f^+_{\beta k}c_{\alpha k}\rangle = (N^{fc}_{\beta\alpha}(k))^*. \tag{2.3b}$$

Thus the distribution function $N$ of the system under consideration is a matrix $N^{ab}_{\alpha\beta}(k)$ with both band indices $a, b = c, f$ and spin indices $\alpha, \beta$. It is convenient to write this matrix in the block form

$$N = \begin{bmatrix} N^c_{\alpha\beta}(k) & N^{cf}_{\alpha\beta}(k) \\ N^{fc}_{\alpha\beta}(k) & N^f_{\alpha\beta}(k) \end{bmatrix}. \tag{2.4}$$

For spin $S = 1/2$, each block is a spin matrix $2\times 2$. According to the general principles of the Landau theory [19] the entropy of a non-equilibrium electron liquid is equal to

$$S(N) = -Sp(N\ln N + (1-N)\ln(1-N)) \tag{2.5}$$

where the trace is taken over all indices. Now we introduce the total energy functional

$$E(N) = \sum_{\alpha k}(\varepsilon(k)N^c_{\alpha\alpha}(k) + \varepsilon_f N^f_{\alpha\alpha}(k)) + \frac{1}{2N_u}\sum_{kp}\sum_{abcd}\sum_{\alpha\beta\gamma\delta} N^{ab}_{\alpha\beta}(k)K^{abcd}_{\alpha\beta\gamma\delta}(k,p)N^{cd}_{\gamma\delta}(p) \tag{2.6}$$

where $N_u$ is the number of unit cells in the lattice. The functional includes different types of interaction. $K^{cccc}_{\alpha\beta\gamma\delta}$ describes potential and exchange interactions between conduction electrons. $K^{ffff}_{\alpha\beta\gamma\delta}$ describes potential and direct exchange interactions between f electrons. $K^{ccff}_{\alpha\beta\gamma\delta}$ and $K^{cffc}_{\alpha\beta\gamma\delta}$ describe potential and exchange interactions between conduction and f electrons. As an investigation of the total energy functional (2.6) is too complicated, we shall study a simpler case when only the exchange interaction between conduction and f electrons is important. Then we have

$$E(N) = \sum_{\alpha k}(\varepsilon(k)N^c_{\alpha\alpha}(k) + \varepsilon_f N^f_{\alpha\alpha}(k)) + \frac{1}{N_u}\sum_{kp}\sum_{\alpha\beta\gamma\delta}(N^f_{\beta\alpha}(k)F_{\alpha\gamma,\beta\delta}(k,p)N^c_{\delta\gamma}(p) + N^{fc}_{\beta\alpha}(k)K_{\alpha\gamma,\beta\delta}(k,p)N^{cf}_{\delta\gamma}(p)) \tag{2.7}$$

where the interaction functions $F$ and $K$ have the following spin structure:

$$F_{\alpha\gamma,\beta\delta}(k,p) = G(k,p)\sigma_{\alpha\beta}\sigma_{\gamma\delta}$$
$$K_{\alpha\gamma,\beta\delta}(k,p) = \varphi(k,p)\delta_{\alpha\beta}\delta_{\gamma\delta} \tag{2.8}$$

where $\sigma^j_{\alpha\beta}$, $j = x, y, z$, are the Pauli matrices. In a general case the interaction function $K_{\alpha\gamma,\beta\delta}(k,p)$ contains a term $K(k,p)\sigma_{\alpha\beta}\sigma_{\gamma\delta}$ which leads to a certain renormalization of magnetic properties.

The free energy of the system has the form

$$\Omega(N) = E(N) - TS(N) - \mu N_t - \lambda N_f. \tag{2.9}$$

The chemical potential $\mu$ determines the total number of conduction and f electrons per unit cell:

$$N_t = \frac{1}{N_u}\sum_{\alpha k}(N^c_{\alpha\alpha}(k) + N^f_{\alpha\alpha}(k)) = \text{constant}. \tag{2.10}$$

The additional chemical potential $\lambda$ determines the number of f electrons per unit cell:

$$N_f = \frac{1}{N_u}\sum_{\alpha k} N^f_{\alpha\alpha}(k) = \text{constant}. \tag{2.11}$$

Actually the parameter $\lambda$ leads to a renormalization of the f-level energy. We define

$$\tilde{\varepsilon}_f = \varepsilon_f - \lambda. \tag{2.12}$$

Therefore it is convenient to define the energy functional in the form

$$\tilde{E}(N) = E(N) - \lambda N_f. \tag{2.13}$$

To find the matrix of quasiparticle energies

$$\varepsilon = \begin{bmatrix} \varepsilon^c_{\alpha\beta}(k) & \varepsilon^{cf}_{\alpha\beta}(k) \\ \varepsilon^{fc}_{\alpha\beta}(k) & \varepsilon^f_{\alpha\beta}(k) \end{bmatrix} \tag{2.14}$$

it is necessary to vary $\tilde{E}(N)$ to $N$. So we obtain

$$\varepsilon^c_{\alpha\beta}(k) = \frac{\delta\tilde{E}}{\delta N^c_{\beta\alpha}(k)} = \varepsilon(k)\delta_{\alpha\beta} + \frac{1}{N_u}\sum_{\gamma\delta p} F_{\alpha\gamma,\beta\delta}(k,p)N^f_{\delta\gamma}(p)$$
$$\varepsilon^f_{\alpha\beta}(k) = \frac{\delta\tilde{E}}{\delta N^f_{\beta\alpha}(k)} = \tilde{\varepsilon}_f\delta_{\alpha\beta} + \frac{1}{N_u}\sum_{\gamma\delta p} F_{\alpha\gamma,\beta\delta}(k,p)N^c_{\delta\gamma}(p) \tag{2.15}$$
$$\varepsilon^{cf}_{\alpha\beta}(k) = \frac{\delta\tilde{E}}{\delta N^{fc}_{\beta\alpha}(k)} = \frac{1}{N_u}\sum_{\gamma\delta p} K_{\alpha\gamma,\beta\delta}(k,p)N^{cf}_{\delta\gamma}(p) = (\varepsilon^{fc}_{\beta\alpha}(k))^*.$$

Minimizing the free energy $\Omega(N)$ with respect to $N$, one obtains the following matrix equation:

$$\delta\Omega(N)/\delta N = \varepsilon - T\delta S/\delta N - \mu\mathbf{1} = 0 \tag{2.16}$$

where $\mathbf{1}$ is the unit matrix with the matrix elements $\delta_{\alpha\beta}\delta_{ab}$. Since $\delta S/\delta N = \ln(N^{-1} - \mathbf{1})$, an equilibrium distribution matrix $N$ has the form

$$N = (\exp((\varepsilon - \mu\mathbf{1})/T) + \mathbf{1})^{-1}. \tag{2.17}$$

The substitution of this solution into (2.15) gives a set of integral equations which enables us to find the matrix of quasiparticle energies (2.14). To determine self-consistently all unknown physical parameters we must take into account equations (2.10) and (2.11).

## 3. Paramagnetic heavy-fermion state

As an example we consider the equilibrium properties of the system in a paramagnetic state. In that case the matrix of quasiparticle energies has a trivial dependence on the spin indices, i.e. $\varepsilon^{ab}_{\alpha\beta} = \varepsilon^{ab}\delta_{\alpha\beta}$ and $N^{ab}_{\alpha\beta} = N^{ab}\delta_{\alpha\beta}$. The substitution of these matrices into (2.15) gives

$$\varepsilon^{c}(k) = \varepsilon(k) \qquad \varepsilon^{f}(k) = \tilde{\varepsilon}_f$$
$$\varepsilon^{cf}(k) = \frac{2}{N_u}\sum_{p}\varphi(k,p)N^{cf}(p) = (\varepsilon^{fc}(k))^*. \tag{3.1}$$

For simplicity we shall study only an isotropic system. In the case of the isotropic Fermi surface, the interaction functions $G(k,p)$ and $\varphi(k,p)$ in (2.8) depend only on the angle $\vartheta$ between the wavenumbers $k$ and $p$. Therefore we can use the expansion in Legendre polynomials:

$$G(k,p) = \sum_{l=0}^{\infty}(2l+1)G_l P_l(\cos\vartheta)$$
$$\varphi(k,p) = \sum_{l=0}^{\infty}(2l+1)\varphi_l P_l(\cos\vartheta). \tag{3.2}$$

As the matrix $N^{ab}$ does not depend on the direction of the wavenumber $k$, the matrix $\varepsilon$ takes the form

$$\varepsilon = \begin{bmatrix} \varepsilon(k) & b \\ b^* & \tilde{\varepsilon}_f \end{bmatrix} \tag{3.3}$$

where we introduce a parameter

$$b = \frac{2\varphi_0}{N_u}\sum_{k} N^{cf}(k). \tag{3.4}$$

Below for simplicity we shall suppose that the parameter $b$ is real, i.e. $b^* = b$. The matrix (3.3) may be written in the diagonal form

$$\varepsilon = U_k^{-1}\begin{bmatrix} E_{1k} & 0 \\ 0 & E_{2k} \end{bmatrix}U_k \tag{3.5}$$

by using a unitary transformation

$$U_k = \begin{bmatrix} \cos\theta_k & -\sin\theta_k \\ \sin\theta_k & \cos\theta_k \end{bmatrix}. \tag{3.6}$$

The angle $\theta_k \in [0,\pi]$ and two quasiparticle energy bands $E_{1k}$ and $E_{2k}$ are determined by the following equations:

$$E_{1k} = \tilde{\varepsilon}_f - b\cot\theta_k = \tfrac{1}{2}(\tilde{\varepsilon}_f + \varepsilon(k) - [(\tilde{\varepsilon}_f - \varepsilon(k))^2 + 4b^2]^{1/2})$$
$$E_{2k} = \tilde{\varepsilon}_f + b\tan\theta_k = \tfrac{1}{2}(\tilde{\varepsilon}_f + \varepsilon(k) + [(\tilde{\varepsilon}_f - \varepsilon(k))^2 + 4b^2]^{1/2}). \tag{3.7}$$

According to (2.17) the distribution function $N$ may be written in the form

$$N = U_k^{-1} \begin{bmatrix} f(E_{1k}) & 0 \\ 0 & f(E_{2k}) \end{bmatrix} U_k \tag{3.8a}$$

where $f(E) = (\exp((E-\mu)/T)+1)^{-1}$. Multiplying the matrices, one obtains

$$\begin{aligned} N^c(k) &= f(E_{1k})\cos^2\theta_k + f(E_{2k})\sin^2\theta_k \\ N^f(k) &= f(E_{1k})\sin^2\theta_k + f(E_{2k})\cos^2\theta_k \\ N^{cf}(k) &= N^{fc}(k) = \tfrac{1}{2}(f(E_{2k}) - f(E_{1k}))\sin(2\theta_k). \end{aligned} \tag{3.8b}$$

Therefore the paramagnetic state of the system is determined completely by three parameters $\mu$, $\tilde{\varepsilon}_f$ and $b$. To find the parameters we must solve three equations (2.10), (2.11) and (3.4). Using the transformation (3.8), they may be written in the form

$$\begin{aligned} N_t &= \frac{2}{N_u}\sum_k (f(E_{1k}) + f(E_{2k})) \\ N_f &= \frac{2}{N_u}\sum_k (f(E_{1k})\sin^2\theta_k + f(E_{2k})\cos^2\theta_k) \\ 1 &= \frac{2\varphi_0}{N_u}\sum_k (f(E_{1k}) - f(E_{2k}))(E_{1k} - E_{2k})^{-1}. \end{aligned} \tag{3.9}$$

In deriving the latter equation we have used a useful equality

$$E_{2k} - E_{1k} = 2b/\sin(2\theta_k). \tag{3.10}$$

The multiplier 2 on the right-hand side of equations (3.9) is a result of summing over two spin states. Comparing equations (3.9) with the mean-field results [5, 21], we find that these equations are completely equivalent to the mean-field equations which describe the coherent Kondo state if the parameter $\varphi_0$ is chosen to be equal to the Kondo coupling energy $J$, i.e. $\varphi_0 = J < 0$. However, it should be noted that, when we use a Landau-like theory to describe a metal, the Landau parameters $\varphi_l$ and $G_l$ must be found from experimental data. The comparison of $J$ with a value of $\varphi_0$ obtained from experimental data can give very interesting information on renormalization of the interaction parameters due to, for example, lattice effects.

It is well known that at $\varphi_0 < 0$ the set of equations (3.9) has a non-trivial solution with $b \neq 0$ at temperatures $T < T_K$. If the total number $N_t$ of electrons is lower than 2, then at $T = 0$ the lower quasiparticle band $E_{1k}$ is partially filled. All calculations may be performed to the end if the conduction band $\varepsilon(k)$ is flat, i.e. $\rho(\varepsilon) = \rho_0$. In that case, at $T = 0$, one obtains the well known results

$$\begin{aligned} T_0 &= \tilde{\varepsilon}_f - \mu = \mu\exp(-1/(2|\varphi_0|\rho_0)) \\ b^2 &= N_f T_0/2\rho_0 \\ m^*/m_0 &= \rho^*/\rho_0 = \cos^{-2}\theta_F = 1 + N_f/2T_0\rho_0 \gg 1 \end{aligned} \tag{3.11}$$

where $\mu \simeq (N_t - N_f)/2\rho_0$ and $T_0\rho_0 \ll 1$. It is the mass enhancement (3.11) that gave them the name 'heavy fermions'. For HF compounds at low temperatures the low-temperature Kondo scale $T_0$ plays the same role as the Fermi temperature in normal metals. The enhancement of the density of states results in a large linear temperature coefficient of the heat capacity $\gamma = 2\pi^2\rho^*/3$. According to (3.11), experimental data for $\gamma$ allow us to determine the Landau parameter $\varphi_0$.

## 4. Magnetic susceptibility

In an external magnetic field $\boldsymbol{H}$ conduction and f electrons obtain additional contributions to their energies $-\frac{1}{2}g_c\mu_B\boldsymbol{H}\sigma$ and $-\frac{1}{2}g_f\mu_B\boldsymbol{H}\sigma$, respectively. Then it is handy to write the matrix of quasiparticle energies (2.15) in the form

$$\begin{aligned}\varepsilon^c_{\alpha\beta}(\boldsymbol{k}) &= \varepsilon(\boldsymbol{k})\delta_{\alpha\beta} - h^c(\boldsymbol{k})\sigma_{\alpha\beta}\\ \varepsilon^f_{\alpha\beta}(\boldsymbol{k}) &= \tilde{\varepsilon}_f\delta_{\alpha\beta} - h^f(\boldsymbol{k})\sigma_{\alpha\beta}\\ \varepsilon^{cf}_{\alpha\beta}(\boldsymbol{k}) &= b(\boldsymbol{k})\delta_{\alpha\beta}\end{aligned} \tag{4.1}$$

where we introduce

$$\begin{aligned}h^c(\boldsymbol{k}) &= \tfrac{1}{2}g_c\mu_B H - \frac{1}{N_u}\sum_{\gamma\delta p} G(\boldsymbol{k},\boldsymbol{p})\sigma_{\gamma\delta}N^f_{\delta\gamma}(\boldsymbol{p})\\ h^f(\boldsymbol{k}) &= \tfrac{1}{2}g_f\mu_B H - \frac{1}{N_u}\sum_{\gamma\delta p} G(\boldsymbol{k},\boldsymbol{p})\sigma_{\gamma\delta}N^c_{\delta\gamma}(\boldsymbol{p})\\ b(\boldsymbol{k}) &= \frac{1}{N_u}\sum_{\gamma p}\varphi(\boldsymbol{k},\boldsymbol{p})N^{cf}_{\gamma\gamma}(\boldsymbol{p}).\end{aligned} \tag{4.2}$$

The parameters $h^c(\boldsymbol{k})$ and $h^f(\boldsymbol{k})$ are the effective magnetic fields which affect conduction and f electrons. They include an additional field produced by surrounding spins owing to the exchange interaction.

Let $\boldsymbol{H}$ be directed along the $z$ axis. It is clear that the effective fields $h^c(\boldsymbol{k})$ and $h^f(\boldsymbol{k})$ are also parallel to the axis. In the isotropic case the parameters $h^c$, $h^f$ and $b$ do not depend on $\boldsymbol{k}$. Using (3.2) we can rewrite equations (4.2) for the $z$ components of the effective field as follows:

$$\begin{aligned}h^c &= \tfrac{1}{2}g_c\mu_B H - \frac{G_0}{N_u}\sum_{\gamma p}\sigma_\gamma N^f_{\gamma\gamma}(\boldsymbol{p})\\ h^f &= \tfrac{1}{2}g_f\mu_B H - \frac{G_0}{N_u}\sum_{\gamma p}\sigma_\gamma N^c_{\gamma\gamma}(\boldsymbol{p})\\ b(\boldsymbol{k}) &= \frac{\varphi_0}{N_u}\sum_{\gamma p}N^{cf}_{\gamma\gamma}(\boldsymbol{p})\end{aligned} \tag{4.3}$$

where $\sigma_\gamma = \pm 1$ for upward and downward spins, respectively. The distribution function $N^{ab}_{\alpha\beta}(\boldsymbol{p})$ is related to the matrix of quasiparticle energies (4.1) by equation (2.17).

The total magnetic moment per unit cell is equal to the sum of magnetic moments of conduction and f electrons:

$$M_t = M_f + M_c = \tfrac{1}{2}g_c\mu_B N_u^{-1}\sum_{\gamma p}\sigma_\gamma N^c_{\gamma\gamma}(\boldsymbol{p}) + \tfrac{1}{2}g_f\mu_B N_u^{-1}\sum_{\gamma p}\sigma_\gamma N^f_{\gamma\gamma}(\boldsymbol{p}). \tag{4.4}$$

Comparing (4.3) and (4.4), one obtains the following useful relation between the fields $h^c$ and $h^f$ and total moment $M_t$:

$$\tfrac{1}{2}g_f\mu_B h^c + \tfrac{1}{2}g_c\mu_B h^f = \tfrac{1}{2}g_c g_f\mu_B^2 H - G_0 M_t. \tag{4.5}$$

Thus we can conclude that in an external magnetic field the equilibrium state is determined completely by five parameters $\mu$, $\varepsilon_f$, $b$, $h^c$ and $h^f$. To find the parameters we must solve the set of the algebraic equations (2.10), (2.11) and (4.3).

First of all we note that, as the effective fields $h^c$ and $h^f$ are parallel to the $z$ axis, the matrix of quasiparticle energies (4.1) and the distribution matrix (2.17) are diagonal matrices with respect to spin indices, i.e. $\varepsilon^{ab}_{\alpha\beta} = \varepsilon^{ab}_{\alpha}\delta_{\alpha\beta}$ and $N^{ab}_{\alpha\beta} = N^{ab}_{\alpha}\delta_{\alpha\beta}$. According to (4.1) the matrix elements $\varepsilon^{ab}_{\alpha}$ have the form

$$\begin{aligned}
&\varepsilon^{c}_{\alpha}(k) = \varepsilon(k) - \sigma_\alpha h^c \\
&\varepsilon^{f}_{\alpha}(k) = \tilde{\varepsilon}_f - \sigma_\alpha h^f \\
&\varepsilon^{cf}_{\alpha}(k) = b.
\end{aligned} \tag{4.6}$$

As the matrix $\varepsilon^{ab}_{\alpha}$ looks like the matrix (3.3), we can transform it to the diagonal form (3.5), using a unitary transformation $U_{k\alpha}$ (3.6). There is only one difference from the case $H = 0$. Namely, at $H \neq 0$, the transformation angle $\theta_{k\alpha}$ depends on the spin index $\alpha$. Generalizing equations (3.7), at $H \neq 0$, we obtain that the quasiparticle energies have the form

$$\begin{aligned}
E_{1k\alpha} &= \tilde{\varepsilon}^f_\alpha - b\cot\theta_{k\alpha} = \tfrac{1}{2}(\tilde{\varepsilon}^f_\alpha + \varepsilon^c_\alpha(k) - [(\tilde{\varepsilon}^f_\alpha - \varepsilon^c_\alpha(k))^2 + 4b^2]^{1/2}) \\
E_{2k\alpha} &= \tilde{\varepsilon}^f_\alpha + b\tan\theta_{k\alpha} = \tfrac{1}{2}(\tilde{\varepsilon}^f_\alpha + \varepsilon^c_\alpha(k) + [(\tilde{\varepsilon}^f_\alpha - \varepsilon^c_\alpha(k))^2 + 4b^2]^{1/2}).
\end{aligned} \tag{4.7}$$

In the same way we generalize equations (3.8) for the distribution matrix $N^{ab}_{\alpha}$. That is, this matrix may be written in the diagonal form (3.8*a*) by using the unitary transformation $U_{k\alpha}$. The matrix elements $N^{ab}_{\alpha}$ are determined by equations (3.8*b*) where we have to replace $E_{1k}$, $E_{2k}$ and $\theta_k$ by $E_{1k\alpha}$, $E_{2k\alpha}$ and $\theta_{k\alpha}$. Substituting these results into equations (2.10), (2.11) and (4.3), we obtain the following complete set of algebraic equations:

$$\begin{aligned}
N_t &= \frac{1}{N_u}\sum_{\alpha k}(f(E_{1k\alpha}) + f(E_{2k\alpha})) \\
N_f &= \frac{1}{N_u}\sum_{\alpha k}(f(E_{1k\alpha})\sin^2\theta_{k\alpha} + f(E_{2k\alpha})\cos^2\theta_{k\alpha}) \\
1 &= \frac{\varphi_0}{N_u}\sum_{\alpha k}(f(E_{1k\alpha}) - f(E_{2k\alpha}))(E_{1k\alpha} - E_{2k\alpha})^{-1} \\
h^c &= \tfrac{1}{2}g_c\mu_B H - \frac{G_0}{N_u}\sum_{\alpha k}\sigma_\alpha(f(E_{1k\alpha})\sin^2\theta_{k\alpha} + f(E_{2k\alpha})\cos^2\theta_{k\alpha}) \\
h^f &= \tfrac{1}{2}g_f\mu_B H - \frac{G_0}{N_u}\sum_{\alpha k}\sigma_\alpha(f(E_{1k\alpha})\cos^2\theta_{k\alpha} + f(E_{2k\alpha})\sin^2\theta_{k\alpha})
\end{aligned} \tag{4.8}$$

which enables us to find the temperature and magnetic field dependences of five unknown parameters $\mu$, $\tilde{\varepsilon}_f$, $b$, $h^c$ and $h^f$ at fixed parameters $N_t$ and $N_f$. Then we can find $M_t(T, H)$ and other physical parameters. Unfortunately in the general case this problem is too difficult. That is why we shall study only the case of low temperatures $T \ll T_0$ and low magnetic fields $\mu_B H \ll T_0$. Solving equations (4.8) becomes simpler if we note that, in accordance with the results in [21], magnetic field corrections to the chemical potential $\mu$, the effective f-level energy $\tilde{\varepsilon}_f$ and the parameter $b$ are second order in $H$. Therefore, in order to study a linear response in a magnetic field, we can neglect the effect of $H$ on $\mu$, $\tilde{\varepsilon}_f$ and $b$. The

problem is reduced to the determination of the effective fields $h^c$ and $h^f$ to first order in $H$. The change in the quasiparticle energies in the external magnetic field $H$ is given by

$$\delta E_{1k\alpha} = E_{1k\alpha} - E_{1k} = \frac{\partial E_{1k}}{\partial \varepsilon(k)} \frac{\partial \varepsilon_\alpha^c(k)}{\partial h^c} h^c + \frac{\partial E_{1k}}{\partial \tilde{\varepsilon}_f} \frac{\partial \varepsilon_\alpha^f}{\partial h^f} h^f + O(H^2)$$
$$= -\sigma_\alpha (h^c \cos^2 \theta_k + h^f \sin^2 \theta_k) + O(H^2) \tag{4.9a}$$

$$\delta E_{2k\alpha} = E_{2k\alpha} - E_{2k} = \frac{\partial E_{2k}}{\partial \varepsilon(k)} \frac{\partial \varepsilon_\alpha^c(k)}{\partial h^c} h^c + \frac{\partial E_{2k}}{\partial \tilde{\varepsilon}_f} \frac{\partial \varepsilon_\alpha^f}{\partial h^f} h^f + O(H^2)$$
$$= -\sigma_\alpha (h^c \sin^2 \theta_k + h^f \cos^2 \theta_k) + O(H^2). \tag{4.9b}$$

Here we have used the equalities

$$\frac{\partial E_{1k}}{\partial \varepsilon(k)} = \frac{\partial E_{2k}}{\partial \tilde{\varepsilon}_f} = \cos^2 \theta_k \qquad \frac{\partial E_{2k}}{\partial \varepsilon(k)} = \frac{\partial E_{1k}}{\partial \tilde{\varepsilon}_f} = \sin^2 \theta_k \tag{4.10}$$

which follow from equations (3.7). As the energy gap between the upper band $E_{2k}$ and the lower band $E_{1k}$ is of the order of $T_0$, at temperatures $T \ll T_0$ we can neglect the occupancy of the upper band, i.e. $f(E_{2k\alpha}) = 0$. The substitution of equations (4.9) into equations (4.8) allows us to write the two latter equations in (4.8) in the form

$$h^c = \tfrac{1}{2} g_c \mu_B H - \frac{G_0}{N_u} \sum_{\alpha k} \sigma_\alpha (f'(E_{1k}) \sin^2 \theta_k \delta E_{1k\alpha} + f(E_{1k}) \delta(\sin^2 \theta_{k\alpha})) \tag{4.11a}$$

$$h^f = \tfrac{1}{2} g_f \mu_B H - \frac{G_0}{N_u} \sum_{\alpha k} \sigma_\alpha (f'(E_{1k}) \cos^2 \theta_k \delta E_{1k\alpha} + f(E_k) \delta(\cos^2 \theta_{k\alpha})) \tag{4.11b}$$

where $f'(E) = \mathrm{d}f(E)/\mathrm{d}E$. Using (4.7), one can easily find that

$$\delta(\sin^2 \theta_{k\alpha}) = -\delta(\cos^2 \theta_{k\alpha}) = \sin^2 \theta_{k\alpha} - \sin^2 \theta_k = \frac{1}{4b} \sigma_\alpha (h^f - h^c) \sin^3(2\theta_k). \tag{4.12}$$

The substitution of equations (4.9) and (4.12) into (4.11) gives a set of linear equations for finding the effective fields $h^f$ and $h^c$:

$$h^c = \tfrac{1}{2} g_c \mu_B H - A h^c - B h^f$$
$$h^f = \tfrac{1}{2} g_f \mu_B H - C h^c - D h^f \tag{4.13}$$

where we introduce the following coefficients:

$$A = D = -\frac{2G_0}{N_u} \sum_k \left( \tfrac{1}{4} f'(E_{1k}) \sin^2(2\theta_k) + \frac{1}{4b} f(E_{1k}) \sin^3(2\theta_k) \right)$$
$$B = -\frac{2G_0}{N_u} \sum_k \left( f'(E_{1k}) \sin^4 \theta_k - \frac{1}{4b} f(E_{1k}) \sin^3(2\theta_k) \right) \tag{4.14}$$
$$C = -\frac{2G_0}{N_u} \sum_k \left( f'(E_{1k}) \cos^4 \theta_k - \frac{1}{4b} f(E_{1k}) \sin^3(2\theta_k) \right).$$

It is not difficult to solve equations (4.13). Then we obtain

$$h^c = \tfrac{1}{2}\mu_B H \frac{(1+A)g_c - Bg_f}{(1+A)^2 - BC}$$
$$h^f = \tfrac{1}{2}\mu_B H \frac{(1+A)g_f - Cg_c}{(1+A)^2 - BC}. \tag{4.15}$$

The coefficients $A$, $B$ and $C$ may be calculated in the case $\rho(\varepsilon) = \rho_0$. For that purpose we use the following transformation from the summation over $k$ to the integration over the energy variable $E = E_{1k}$:

$$\frac{1}{N_u}\sum_k = \int d\varepsilon\, \rho(\varepsilon) = \rho_0 \int \frac{dE}{\cos^2\theta_k} \tag{4.16}$$

where the function $\cos^2\theta_k$ has to be considered as a function of the variable $E = E_{1k}$. One can prove the following equalities:

$$A = -2G_0\rho_0 \int_{E_{min}}^{E_{max}} dE \frac{d}{dE}(f(E)\sin^2\theta_k) = -2G_0\rho_0 b^2 \frac{f(E)}{(\tilde{\varepsilon} - E)^2 + b^2}\bigg|_{E_{min}}^{E_{max}} \tag{4.17a}$$

$$A + C = -2G_0\rho_0 \int_{E_{min}}^{E_{max}} dE\, f'(E) = 2G_0\rho_0(f(E_{min}) - f(E_{max})) \tag{4.17b}$$

$$B + C = -2G_0\rho_0 \int_{E_{min}}^{E_{max}} dE\, f'(E)\tan^2\theta_k \tag{4.17c}$$

where $E_{min}$ and $E_{max}$ are the energies of the bottom and top of the lower quasiparticle band $E_{1k}$.

First of all we shall discuss the magnetic properties at zero temperature. In this case we have $f(E_{min}) = 1$, $f(E_{max}) = 0$, $f'(E) = -\delta(E - \mu)$ and $(\tilde{\varepsilon}_f - E_{min})^2 \approx \mu^2$. Since $\mu \gg b$, equations (4.17) give

$$A = 2G_0\rho_0(b/\mu)^2$$
$$C = 2G_0\rho_0(1 - (b/\mu)^2) \simeq 2G_0\rho_0 \tag{4.18}$$
$$B = 2G_0\rho_0(\tan^2\theta_F - 1 + (b/\mu)^2) \simeq G_0 N_f/T_0$$

where we have used the results (3.11) for the parameters $b$ and $\cos^2\theta_F$ and the inequality $b^2/\mu^2 \sim T_0\rho_0 \ll 1$. It is natural to suppose that the Landau parameter $G_0$ which characterizes the antiferromagnetic interaction between conduction and f electrons, is much smaller than the conduction band width, i.e. $G_0\rho_0 \ll 1$. However, the ratio $G_0/T_0$ is of arbitrary values. So the coefficients $A$, $B$ and $C$ satisfy the inequalities

$$A \ll C \ll B \qquad A \ll 1 \qquad C \ll 1. \tag{4.19}$$

It is important to note that these inequalities are also valid at nonzero temperatures. Using the results (4.18), we can find the fields $h^c$ and $h^f$ at $T = 0$:

$$h^c = \tfrac{1}{2}g_c\mu_B H \frac{1 - N_f g_f G_0/T_0 g_c}{1 - T_m/T_0}$$
$$h^f = \tfrac{1}{2}g_f\mu_B H \frac{1}{1 - T_m/T_0} \tag{4.20}$$

where we introduce the parameter

$$T_m = 2N_f G_0^2 \rho_0. \tag{4.21}$$

The physical meaning of $T_m$ will be discussed briefly below. The result (4.20) has interesting physical features. Let us consider the region of the Landau parameters $\varphi_0$ and $G_0$ where $T_0 > T_m$ but $G_0 > T_0 g_c / N_f g_f \sim T_0$. This region is sufficiently broad. Specifically it includes the values $G_0 \sim |\varphi_0| \sim |J|$. In this region the effective field $h^f$ is positive and $h^c$ is negative. This means that, while $h^f$ is parallel to the external magnetic field $H$, the field $h^c$ is antiparallel to $H$. This result becomes clear if we note that it is brought about by the antiferromagnetic exchange interaction (2.8) between conduction and f electrons. In the external magnetic field $H$, f electrons are arranged parallel to this field. Spins of conduction electrons are also parallel to $H$ if the antiferromagnetic interaction with f electrons is neglected. The antiferromagnetic interaction tries to overturn conduction electron spins. At $G_0 > T_0$ the state with downward conduction electron spins is energetically more favourable.

In order to find the total magnetic moment $M_t$ we substitute equations (4.15) into equality (4.5), taking into account inequality (4.19). Simple calculations give

$$M_t = \tfrac{1}{4} g_f^2 \mu_B^2 H \frac{B}{G_0(1 - BC)}. \tag{4.22}$$

Therefore the magnetic susceptibility is

$$\chi = \frac{dM_t}{dH} = \tfrac{1}{4} g_f^2 \mu_B^2 \frac{B}{G_0(1 - BC)}. \tag{4.23}$$

As at $T = 0$ the coefficients $B$ and $C$ are determined by equations (4.18), we obtain

$$\chi(0) = \tfrac{1}{4} g_f^2 \mu_B^2 N_f \frac{1}{T_0 - T_m}. \tag{4.24}$$

In the case when $G_0 = 0$ we have $T_m = 0$. Then equation (4.24) coincides with the mean-field results [5] for zero-temperature susceptibility of HF compounds. At nonzero $G_0$ the result (4.24) has been obtained in [22] on the basis of an extended Coqblin–Schrieffer model which enables us to take into account the RKKY interaction.

Let us discuss the result (4.23). As the susceptibility must be positive, the paramagnetic HF state is stable only in the region of the Landau parameters $\varphi_0$ and $G_0$ where $T_0 > T_m$. The physical meaning of the parameter $T_m$ becomes clear if we note that according to a microscopic approach the parameter $T_m$ is the characteristic energy of the RKKY interaction mediated by conduction electrons between localized f spins. This enables us to understand the origin of the instability at $T_0 = T_m$. That is, in the region $T_0 < T_m$ the RKKY interaction is strong enough to break the coherent HF state. At $T = 0$ a stable-moment state with long-range magnetic order is formed. In this region of the Landau parameters the Kondo effect is incoherent at all temperatures including $T = 0$. This problem has been discussed in many papers (see, for example, [1, 3, 22], and references therein). In the framework of our phenomenological approach this means that the wavefunctions of quasiparticles near the Fermi surface are not equal to the wavefunctions (2.2). Then the non-diagonal matrix elements $N^{ab}$ of the distribution matrix are equal to zero at all temperatures. In that case our phenomenological theory becomes equivalent to the usual Landau Fermi-liquid theory of two band models (see, for example, [18]).

## 5. Ferromagnetic phase transition

According to equation (4.23) the temperature dependence of the magnetic susceptibility $\chi$ is determined by the parameters $B$ and $C$. Equations (4.17*a*) and (4.17*b*) show that the temperature dependence of $C$ is exponentially weak, i.e. $C = 2G_0\rho_0 + O(\exp(-\mu/T))$. To find the temperature dependence of $B$ we must calculate the integral (4.17*c*). As $\tan^2\theta_k = b^2/(\tilde{\varepsilon} - E)^2$ and $C \ll B$, at $T \ll T_0$ we obtain

$$B = 2G_0\rho_0 b^2(\tilde{\varepsilon}_f - \mu)^{-2}(1 + \pi^2T^2(\tilde{\varepsilon} - \mu)^{-2}) + O(T^4/T_0^4). \tag{5.1}$$

According to [21] the parameters $\tilde{\varepsilon}_f$ and $b$ have the following temperature dependences:

$$b = b(0)\left(1 - \frac{\pi^2}{12}\left(\frac{T}{T_0}\right)^2\right)$$

$$\tilde{\varepsilon}_f - \mu = T_0\left(1 + \frac{\pi^2}{6}\left(\frac{T}{T_0}\right)^2\right). \tag{5.2}$$

This enables us to find $B$:

$$B = G_0N_fT_0^{-1}\left(1 + \frac{\pi^2}{2}\left(\frac{T}{T_0}\right)^2\right). \tag{5.3}$$

Consequently the magnetic susceptibility (4.23) is given by

$$\chi(T) = \tfrac{1}{4}g_f^2\mu_B^2N_f\left(1 + \frac{\pi^2}{2}\left(\frac{T}{T_0}\right)^2\right)\left(T_0 - T_m - \frac{\pi^2}{2}T_m\left(\frac{T}{T_0}\right)^2\right)^{-1}. \tag{5.4}$$

Let $T_0$ be slightly larger than $T_m$, i.e. $0 < T_0 - T_m \ll T_0$. As we have discussed above, at $T = 0$ the system is in the paramagnetic HF state. However, with increasing temperature the susceptibility increases and diverges at the critical temperature

$$T_c = \frac{\sqrt{2}}{\pi}T_0\left(\frac{T_0}{T_m} - 1\right)^{1/2} \ll T_0. \tag{5.5}$$

This singularity gives evidence of a ferromagnetic instability of the paramagnetic HF state. Let us show that at $T > T_c$ the ferromagnetism and coherent HF state coexist. This means that both the spontaneous magnetic moment and the parameter $b$ in (4.3) are nonzero. It is obvious that the spontaneous magnetic moments of conduction and f electrons are related to the rise in spontaneous effective fields $h^c$ and $h^f$ (4.3) at zero external magnetic field. Therefore we face the following problem. Is there a nontrivial solution of equations (4.8) with nonzero parameters $b$, $h^c$ and $h^f$ at temperatures $T > T_c$ and $H = 0$? To first order in $h^c$ and $h^f$, equations (4.8) are reduced to equations (4.13). These equations have a nontrivial solution above a certain critical temperature at which the determinant of the set of the equations is equal to zero. Taking into account the inequality (4.19), this condition may be written in the form

$$1 - BC = 0 \tag{5.6}$$

which is completely equivalent to the divergency condition of the susceptibility of the magnetic susceptibility (4.23) or (5.4). Consequently, in a certain temperature interval above $T_c$ the coexistence of long-range ferromagnetic order and the coherent HF state is possible. Such a ferromagnetic HF state has been previously discussed in the framework of an extended Coqblin–Schrieffer model [22]. Of course with increasing temperature above a certain critical temperature the ferromagnetic order is broken and the system undergoes a phase transition into a paramagnetic state.

## 6. Discussion and conclusions

In the present paper we have generalized the Landau Fermi-liquid theory for describing electrons in HF compounds. Our phenomenological theory has been based on two assumptions. First we have supposed that the quasiparticle wavefunctions near the Fermi surface are superpositions of the wavefunctions of conduction and f electrons. This assumption has enabled us to introduce the distribution matrix $N_{\alpha\beta}^{ab}(k)$ with both the band indices $a, b = c, f$ and spin indices $\alpha, \beta$. The diagonal elements $N_{\alpha\beta}^{aa}(k)$ describe the distribution of electrons over states in the conduction band and narrow f band. The nondiagonal elements $N_{\alpha\beta}^{cf}(k)$ and $N_{\alpha\beta}^{fc}(k)$ describe the formation of a phase coherence between electron states in the bands, which is the main assumption of the mean-field approach [5, 10–12]. That is why good agreement between our phenomenological theory and the mean-field approach is natural. The correspondence between the mean-field approximation and the Landau-like Fermi liquid theory of several magnetic impurity models has been discussed in detail in [23] where it has been shown that the application of the mean-field theory to these models gives asymptotically exact results at $T \to 0$ and $H \to 0$.

Secondly we have assumed that the number of f electrons is fixed. We have introduced this condition by using an additional chemical potential of f electrons that actually results in a renormalization of the f-level energy. On the basis of an exact microscopic approach to the periodic Anderson model in the limiting case $U \to \infty$ and $\mu - \varepsilon_f \gg \pi|V|^2\rho_0$, fixing the f-level occupancy is imposed by special constraints on each f ion. However, in the mean-field approximation [5, 10, 11] the constraints are also replaced by fixing the total number of f electrons using an additional chemical potential.

Although our Landau-like Fermi-liquid approach and mean-field approach based on large-degeneracy models have a general basis, there are some significant differences. So far the account of the RKKY interaction in the framework of the $1/N$ expansion applied to the conventional slave boson or Coqblin–Schrieffer models is an unsolved problem because it demands taking into account higher orders of the $1/N$ expansion. The problem may be partly solved by using an extended Coqblin–Schrieffer model which enables the magnetism of HF compounds to be described [23]. Nevertheless these difficulties restrict significantly possibilities of the mean-field approach for describing magnetic phase transitions. Unlike that approach, our Landau-like Fermi-liquid theory allows us to take into account, on the same basis, different types of interaction, including magnetic interactions. In order to show this, we have studied the ferromagnetic instability of HF compounds. It has been found that at $T = 0$ the coexistence of ferromagnetism and the coherent HF state is impossible. It becomes possible in a certain temperature range above zero temperature if the system is sufficiently close to the ferromagnetic instability. Moreover the Landau Fermi-liquid approach may be used for describing kinetic and relaxation phenomena in HF compounds. This problem will be studied in a forthcoming paper.

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