Phenomenological Fermi-liquid theory of heavy-fermion compounds

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A phenomenological Fermi-liquid theory has been developed for describing the low-temperature properties of heavy-fermion compounds. The theory predicts results which agree completely with those found by microscopic approaches.© *1995 American Institute of Physics.*

The unusual thermodynamic and kinetic properties of heavy-fermion compounds stem from strong electron correlations, specifically, an interaction of conduction electrons with the magnetic moments of ions of rare earth elements or uranium which have a partially filled f shell (see, for example, a review[1]). At temperatures T above the Kondo temperature T_K, this interaction leads to the Kondo effect, i.e., a magnetic screening of the localized moments by conduction electrons. The screening occurs independently at each magnetic ion (this is an incoherent Kondo effect). At low temperatures, $T<T_K$, the Kondo effect becomes coherent and gives rise to a nonmagnetic ground state. Quasiparticle states near the Fermi surface have an anomalously large mass $m^*/m_0 \sim 10^2$. According to experimental data, the electrons behave as a normal Fermi liquid at $T \ll T_K$. Competing with the Kondo effect is the RKKY exchange interaction, which can partially or completely disrupt the Kondo screening and give rise to a magnetically ordered phase.

In this letter we generalize Landau's phenomenological Fermi-liquid theory[2,3] to the case of electrons in heavy-fermion compounds. We first give a general formulation of the phenomenological approach, and then look at thermal and magnetic properties of heavy-fermion compounds at $T \ll T_K$. In particular, we examine how the RKKY interaction affects the magnetic susceptibility of these compounds and the problem of the coexistence of a coherent Kondo effect and a ferromagnetism. Nozières[4] has previously derived a phenomenological Fermi-liquid approach for describing electrons in the single-impurity Kondo model. The results agree well with an exact solution.[5]

In this letter we consider a system which can be described by Anderson's lattice model. The system consists of conduction electrons in an energy band $\epsilon(\mathbf{k})$ and f electrons in a very narrow band, whose dispersion we ignore. We are thus actually dealing with an f level with an energy $\epsilon_f < \mu$, where μ is the chemical potential. Because of the strong single-site Coulomb repulsion U_0, a double filling of the f level is unfavorable from the energy standpoint. An interaction between conduction electrons and f electrons results from a hybridization of f states and conduction-band states. In the limit

$\mu - \epsilon_f \gg 0$, $U_0 \to 0$, the interaction of the spin of the electron (S_f) with the local spin density of the conduction electrons (S_c) is described by the Kondo Hamiltonian $H = -JS_fS_c$, where J is the energy of the antiferromagnetic exchange interaction ($J<0$). In this case the number of f electrons in the ϵ_f level is on the order of one and is a weak function of the temperature.

Our phenomenological approach starts from two assumptions. First, we assume that the wave function of the quasiparticles near the Fermi surface at $T \ll T_K$ is a superposition of Bloch wave functions of electron states in the conduction band and the narrow f band:

$$\Psi_\alpha(\mathbf{k}) = A_{\alpha\mathbf{k}}\Psi^c_\alpha(\mathbf{k}) + B_{\alpha\mathbf{k}}\Psi^f_\alpha(\mathbf{k}), \tag{1}$$

where α is the spin index of a spin $s = 1/2$. Second, we assume that, for a fixed filling of the f level, we can introduce an additional chemical potential λ and thereby incorporate a Hubbard repulsion U_0. These assumptions can be justified only within the framework of the mean-field theory[6] or Guzwiller's variational approach.[7]

We introduce a distribution function, which in our case is a matrix in the spin indices (α,β) and the band indices (c,f):

$$N = \begin{pmatrix} N^C_{\alpha\beta}(\mathbf{k}) & N^{cf}_{\alpha\beta}(\mathbf{k}) \\ N^{fc}_{\alpha\beta}(\mathbf{k}) & N^f_{\alpha\beta}(\mathbf{k}) \end{pmatrix}. \tag{2}$$

The diagonal elements of this matrix describe the momentum distribution of the electrons in the conduction band and in the f band. Off-diagonal elements N^{cf} and N^{fc} are introduced here because of assumption (1). According to the general principles of Landau's theory,[8] the entropy of a nonequilibrium electron liquid is

$$S(N) = -\,\mathrm{Tr}[N\ln N + (1-N)\ln(1-N)]. \tag{3}$$

We define an energy functional which incorporates only the exchange interaction between conduction electrons and f electrons:

$$E(N) = \sum_{\alpha\mathbf{k}} [\epsilon(\mathbf{k})N^c_{\alpha\alpha}(\mathbf{k}) + \epsilon_f N^f_{\alpha\alpha}(\mathbf{k})]$$

$$+ \frac{1}{N_u}\sum_{\mathbf{kp}}\sum_{\alpha\beta\gamma\delta} + [N^f_{\beta\alpha}(\mathbf{k})F_{\alpha\gamma,\beta\delta}(\mathbf{k},\mathbf{p})N^c_{\delta\gamma}(\mathbf{p}) + N^{fc}_{\beta\alpha}(\mathbf{k})K_{\alpha\gamma,\beta\delta}(\mathbf{k},\mathbf{p})N^{cf}_{\delta\gamma}(\mathbf{p})], \tag{4}$$

where N_u is the number of unit cells in the system,

$$F_{\alpha\gamma,\beta\delta}(\mathbf{k},\mathbf{p}) = G(\mathbf{k},\mathbf{p})\sigma_{\alpha\beta}\,\sigma_{\gamma\delta}, \quad \text{and} \quad K_{\alpha\gamma,\beta\delta}(\mathbf{k},\mathbf{p}) = \varphi(\mathbf{k},\mathbf{p})\,\delta_{\alpha\beta}\delta_{\gamma\delta}. \tag{5}$$

We will consider only the isotropic case. For values of $\mathbf{k}$ and $\mathbf{p}$ which lie on the Fermi surface, we can thus expand the functions $G(\mathbf{k},\mathbf{p})$ and $\varphi(\mathbf{k},\mathbf{p})$ in series in Legendre polynomials:

$$G(\mathbf{k},\mathbf{p}) = \sum_{l=0}^{\infty}(2l+1)G_lP_l(\cos\nu), \quad \varphi(\mathbf{k},\mathbf{p}) = \sum_{l=0}^{\infty}(2l+1)\varphi_lP_l(\cos\nu). \tag{6}$$

The free energy of the system is

$$\Omega(N) = E(N) - TS(N) - \mu N_t - \lambda N_f. \tag{7}$$

The chemical potential μ is determined by the specification of the total number of electrons in one unit cell, N_t:

$$N_t=\frac{1}{N_u}\sum_{\alpha\mathbf{k}}[N^c_{\alpha\alpha}(\mathbf{k})+N^f_{\alpha\alpha}(\mathbf{k})]=\text{const.} \tag{8}$$

We define the additional chemical potential λ by specifying the number of f electrons:

$$N_f=\frac{1}{N_u}\sum_{\alpha\mathbf{k}}N^f_{\alpha\alpha}(\mathbf{k})=\text{const.} \tag{9}$$

The parameter λ renormalizes the energy of the f level: $\epsilon^*_f=\epsilon_f-\lambda$. It is thus convenient to define an energy functional by $E^*(N)=E(N)-\lambda N_f$. A variation of $E^*(N)$ with respect to N yields a matrix of quasiparticle energies ϵ with the components

$$\epsilon^c_{\alpha\beta}(\mathbf{k})=\frac{\delta E^*}{\delta N^c_{\beta\alpha}(\mathbf{k})}=\epsilon(\mathbf{k})\delta_{\alpha\beta}+\frac{1}{N_u}\sum_{\gamma\delta\mathbf{p}}F_{\alpha\gamma,\beta\delta}(\mathbf{k},\mathbf{p})N^f_{\delta\gamma}(\mathbf{p}),$$

$$\epsilon^f_{\alpha\beta}(\mathbf{k})=\frac{\delta E^*}{\delta N^f_{\beta\alpha}(\mathbf{k})}=\epsilon^*_f\delta_{\alpha\beta}+\frac{1}{N_u}\sum_{\gamma\delta\mathbf{p}}F_{\alpha\gamma,\beta\delta}(\mathbf{k},\mathbf{p})N^c_{\delta\gamma}(\mathbf{p}),$$

$$\epsilon^{cf}_{\alpha\beta}(\mathbf{k})=\frac{\delta E^*}{\delta N^{fc}_{\beta\alpha}(\mathbf{k})}=\frac{1}{N_u}\sum_{\gamma\delta\mathbf{p}}K_{\alpha\gamma,\beta\delta}(\mathbf{k},\mathbf{p})N^{cf}_{\delta\gamma}(\mathbf{p}), \tag{10}$$

Variation of free energy (7) with respect to N leads to the variational equation

$$\epsilon-\mu\hat{1}=T\ln(N^{-1}-\hat{1}), \tag{11}$$

where $\hat{1}$ is the unit matrix. Substituting (10) into (11), we find an integral equation for N.

Let us consider the solution of these equations for a paramagnetic state. In this case we seek a solution in a form which is independent of the spin: $\epsilon_{\alpha\beta}=\epsilon\delta_{\alpha\beta}$, $N_{\alpha\beta}=N\delta_{\alpha\beta}$. The matrix ϵ can be written in the form

$$\epsilon=\begin{pmatrix}\epsilon(\mathbf{k}) & b\\ b^* & \epsilon^*_f\end{pmatrix}, \tag{12}$$

where we have introduced the parameter

$$b=\frac{2\varphi_0}{N_u}\sum_{\mathbf{k}}N^{cf}(\mathbf{k}), \tag{13}$$

which we assume for simplicity is real. The matrix of quasiparticle energies ϵ can be put in diagonal form by the unitary transformation $\mathcal{U}$:

$$\epsilon=\mathcal{U}^{-1}\begin{pmatrix}E_1(k) & 0\\ 0 & E_2(k)\end{pmatrix}\mathcal{U},\quad \mathcal{U}=\begin{pmatrix}\cos\theta_{\mathbf{k}} & -\sin\theta_{\mathbf{k}}\\ \sin\theta_{\mathbf{k}} & \cos\theta_{\mathbf{k}}\end{pmatrix}. \tag{14}$$

The diagonal elements are quasiparticle energies:

$$E_1(\mathbf{k}) = \epsilon_f^* - b\cot\theta_{\mathbf{k}} = \tfrac{1}{2}(\epsilon_f^* + \epsilon(\mathbf{k}) - \{[\epsilon_f^* - \epsilon(\mathbf{k})]^2 + 4b^2\}^{1/2}),$$

$$E_2(\mathbf{k}) = \epsilon_f^* + b\tan\theta_{\mathbf{k}} = \tfrac{1}{2}(\epsilon_f^* + \epsilon(\mathbf{k}) + \{[\epsilon_f^* - \epsilon(\mathbf{k})]^2 + 4b^2\}^{1/2}). \tag{15}$$

Using (11), we can also write the distribution function N in diagonal form: $N = \mathcal{U}^{-1} N_d \mathcal{U}$, with diagonal elements $N_d^c = f[E_1(\mathbf{k})]$ and $N_d^f = f[E_2(\mathbf{k})]$, where $f(E) = \{\exp[(E-\mu)/T+1]^{-1}$. Substituting this solution for N into Eqs. (8), (9), and (13), we find the following complete, self-consistent system of equations:

$$N_t = \frac{2}{N_u}\sum_{\mathbf{k}} \{f[E_1(\mathbf{k})] + f[E_2(\mathbf{k})]\},$$

$$N_f = \frac{2}{N_u}\sum_{\mathbf{k}} \{f[E_1(\mathbf{k})]\sin^2\theta_{\mathbf{k}} + f[E_2(\mathbf{k})]\cos^2\theta_{\mathbf{k}}\},$$

$$1 = (2\varphi_0/N_u)\sum_{\mathbf{k}} \{f[E_1(\mathbf{k})] - f[E_2(\mathbf{k})]\}/[E_1(\mathbf{k}) - E_2(\mathbf{k})]. \tag{16}$$

Using this system of equations we can determine three independent parameters: the chemical potential μ, the renormalized f-level energy ϵ_f^*, and b. Comparing Eqs. (16) with the results of Ref. 6, we easily see that these equations are completely the same as the equations of mean-field theory if we set the interaction parameter φ_0 equal to the exchange-interaction energy J. We assume that the total number of electrons is $N_t < 2$; at $T = 0$ the ground state is then characterized by the parameters

$$T_0 \equiv \epsilon_f^* - \mu = \mu\exp(-1/2|\varphi_0|\rho_0), \quad b = (N_f T_0/2\rho_0)^{1/2}. \tag{17}$$

The effective mass of the quasiparticles in the lower band, $E_1(\mathbf{k})$, and the density of states ρ^* near the Fermi surface are considerably larger than the initial parameters: $m^*/m_0 = \rho^*/\rho_0 = 1 + N_f/2T_0\rho_0 \gg 1$, where ρ_0 is the density of states in the $\epsilon(\mathbf{k})$ band. In turn, an increase in the density of states leads to an increase in the linear specific heat $\gamma = 2\pi^2\rho^*/3$.

Let us examine the magnetic properties of a heavy-fermion compound from the phenomenological standpoint. In an external magnetic field H_0 directed along the z axis, the conduction electrons and f electrons with spin $\pm 1/2$ acquire energies $\mp g_c\mu_B H_0/2$ and $\mp g_f\mu_B H_0/2$, respectively. Solving Eqs. (8)–(11), we find that the static magnetic susceptibility at $T = 0$ is

$$\chi = g_f^2\mu_B^2 N_f/4(T_0 - T_m), \tag{18}$$

where the parameter T_m is $2N_f G_0^2\rho_0$. The susceptibility χ is dominated by the f electrons. To see the physical meaning of the parameter T_m, we note that it stems from the exchange interaction between f electrons and conduction electrons. This interaction leads to the RKKY indirect exchange interaction between the spins of localized f electrons. It is a straightforward matter to show that the parameter T_m is a characteristic energy of the RKKY interaction. According to (18), the RKKY interaction increases the magnetic susceptibility and leads to an instability of the heavy-fermion state with respect to magnetism. For parameter values $T_0 < T_m$ the ground state of the system is magnetically

ordered, and the Kondo effect is completely suppressed. This condition becomes the same as the generally accepted condition, which is discussed in Ref. 1, among other places, if we set the parameter G_0 proportional to the energy J. If $T_0 > T_m$, the system is in a paramagnetic heavy-fermion state at $T=0$. At $T=0$, there thus cannot be a coexistence of a ferromagnetism and a coherent Kondo effect. Such a coexistence does become possible at $T \neq 0$, if the low-temperature Kondo scale T_0 in (17) is a bit higher than T_m. Analysis of the temperature dependence of the magnetic susceptibility, $\chi(T)$, shows that as the temperature is raised from zero, the susceptibility $\chi(T)$ increases, and it diverges at a critical temperature $T_c = (\sqrt{2}/\pi)T_0(T_0/T_m - 1)^{1/2}$. This divergence is an indication of a ferromagnetic transition. At $T > T_c$, a ferromagnetic heavy-fermion state forms. In this state the coherent Kondo effect is only partially—not completely—suppressed ($b \neq 0$). As the temperature is raised further, above a certain critical temperature T_c^*, the ferromagnetic order is disrupted, and the system goes back into a paramagnetic state, but now with an incoherent Kondo effect. A similar scenario for the temperature dependence was recently discussed on the basis of a microscopic theory in Ref. 9.

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