Macroscopic theory of transport phenomena in heavy-fermion compounds

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The Landau–Silin equation is extended to describe electronic transport phenomena in heavy-fermion compounds. The macroscopic dielectric response is studied on the basis of this approach. © *1995 American Institute of Physics.*

Electrons in heavy-fermion compounds (HFCs) are an example of a coherent Fermi liquid. At tempeartures below the Kondo temperature T_0 a coherent electronic state is formed because of the Kondo effect. This situation is manifested in both the thermodynamic and transport properties of heavy-fermion compounds.[1]

In our preceding study,[2] we developed a macroscopic description of the thermodynamic properties of HFCs on the basis of a generalized Landau theory. In the present paper we propose a macroscopic description of transport phenomena in HFCs. As an example of the application of this phenomenological approach, we shall investigate the dielectric response. Specifically, we shall consider plasma oscillations and screening of the charge.

According to Ref. 2 , the macroscopic description of the properties of HFCs on the basis of the Landau theory[3,4] is based on two assumptions: 1) Near the Fermi surface the wave function of the quasiparticles is a superposition of Bloch wave functions of the electrons in a wide conduction band $\epsilon(\mathbf{k})$ and narrow f band (we ignore the dispersion of the latter band and actually assume a narrow level); 2) the number of f electrons at the f level is fixed. The first assumption characterizes the formation of a coherent Kondo state. As a result, the electron distribution is described by a matrix distribution function $N^{ab}_{\alpha\beta}(\mathbf{k})$, which contains the band indices a and b, which assume the values c and f, and the spin indices α and β for spin 1/2:

$$N=\begin{pmatrix} N^{c}_{\alpha\beta}(\mathbf{k}) & N^{cf}_{\alpha\beta}(\mathbf{k}) \\ N^{fc}_{\alpha\beta}(\mathbf{k}) & N^{f}_{\alpha\beta}(\mathbf{k}) \end{pmatrix}. \tag{1}$$

The diagonal elements $N^{c}_{\alpha\beta}(\mathbf{k})$ and $N^{f}_{\alpha\beta}(\mathbf{k})$ describe the electron distribution in the conduction band in the f band, respectively. The off-diagonal elements $N^{cf}_{\alpha\beta}(\mathbf{k}) = [N^{fc}_{\alpha\beta}(\mathbf{k})]^*$ characterize coherent phenomena in HFCs. Another important concept of the theory is the matrix of quasiparticle energies $\epsilon^{ab}_{\alpha\beta}(\mathbf{k})$, which in the paramagnetic state has the form

$$\epsilon(\mathbf{k})=\delta_{\alpha\beta}\begin{pmatrix} \epsilon(\mathbf{k}) & b \\ b^* & \epsilon_f \end{pmatrix}, \tag{2}$$

where $\epsilon(\mathbf{k})$ is the energy of electrons in the conduction band, and ϵ_f is the effective energy of the f level, determined from the condition that the f band is filled with N_f electrons: $N_f=\Sigma_{\alpha\mathbf{k}}N^f_{\alpha\alpha}(\mathbf{k})$. The coherence parameter b is determined by the relation $b=\Sigma_{\alpha\mathbf{p}}\varphi(\mathbf{k},\mathbf{p})N^{cf}_{\alpha\alpha}(\mathbf{p})$. In general, this is a complex number. We restrict the discussion to the case $\varphi(\mathbf{k},\mathbf{p})=\varphi_0=$ const, where the parameter b does not depend on $\mathbf{k}$.

We now consider the deviation of the distribution function from the equilibrium value N_0: $N(\mathbf{k},\mathbf{r},t)=N_0(\mathbf{k})+N_1(\mathbf{k},\mathbf{r},t)$. This changes the matrix of quasiparticle energies: $\epsilon(\mathbf{k},\mathbf{r},t)=\epsilon_0(\mathbf{k})+\epsilon_1(\mathbf{k},\mathbf{r},t)$. In the paramagnetic state we have

$$\epsilon_1(\mathbf{k},\mathbf{r},t)=\delta_{\alpha\beta}\begin{pmatrix}0 & b_1(\mathbf{r},t)\\ b_1^*(\mathbf{r},t) & \epsilon_f(\mathbf{r},t)\end{pmatrix}. \tag{3}$$

According to Eq. (3), the matrix element ϵ_1^c is zero, which is a consequence of the fact that only the exchange interaction between the electrons is taken into account. In general, the fluctuations of the complex function $b_1(\mathbf{r},t)$ describe fluctuations of the modulus and phase of the coherence parameter. It is important to note that ϵ_1 is independent of $\mathbf{k}$.

On the basis of Landau's theory (see, for example, Refs. 5 and 6) the nonequilibrium distribution function N is described by the transport equation

$$\partial N/\partial t+\{\nabla_{\mathbf{r}}N\nabla_{\mathbf{k}}\epsilon\}-\{\nabla_{\mathbf{k}}N\nabla_{\mathbf{r}}\epsilon\}-i[\epsilon,N]=I(N_1), \tag{4}$$

where $I(N_1)$ is a collision integral, and $2\{AB\}=AB+BA$. Linearizing Eq. (4), we obtain

$$\partial N_1/\partial t+\{\nabla_{\mathbf{r}}N_1\nabla_{\mathbf{k}}\epsilon_0\}-\{\nabla_{\mathbf{k}}N_0\nabla_{\mathbf{r}}\epsilon_1\}-i[\epsilon_1,N_0]-i[\epsilon_0,N_1]=I(N_1). \tag{5}$$

We now sum (5) over all $\mathbf{k}$ and take the trace over the band and spin indices. Since the contribution of the colllision integral is zero, and since the matrix ϵ_1, according to Eq. (3), does not depend on $\mathbf{k}$, we obtain at the continuity equation

$$\partial\mathcal{N}/\partial t+\operatorname{div}\mathbf{J}=0, \tag{6}$$

which relates the change in the concentration of the total number of electrons, $\mathcal{N}=\Sigma_{\alpha\mathbf{k}}(N^c_{\alpha\alpha}+N^f_{\alpha\alpha})$, to the particle flux

$$\mathbf{J}=\sum_{\alpha\mathbf{k}}\mathbf{v}_{0\mathbf{k}}N^c_{1\alpha\alpha}(\mathbf{k},\mathbf{r},t). \tag{7}$$

Here $\mathbf{v}_{0\mathbf{k}}=\nabla_{\mathbf{k}}\epsilon(\mathbf{k})$ is the renormalized velocity of the conduction electrons. From the physical standpoint, this result follows from the fact that the f electrons are localized and the flux is produced by the motion of the conduction electrons. We note that if the amplitude of the interaction $\varphi(\mathbf{k},\mathbf{p})$ is not constant, then the expression for the flux contains additional terms. This problem, however, falls outside the scope of the present paper.

The kinetic equation (4) must be supplemented by two additional equations:

$$\sum_{\alpha\mathbf{k}}N^f_{1\alpha\alpha}(\mathbf{k},\mathbf{r},t)=0, \tag{8}$$

$$\varphi_0\sum_{\alpha\mathbf{k}}N^{cf}_{1\alpha\alpha}(\mathbf{k},\mathbf{r},t)=b_1(\mathbf{r},t). \tag{9}$$

Equation (8) means that the number of f electrons is fixed and does not depend $\mathbf{r}$ and t. Equation (9) relates the fluctuations of the coherence parameter $b(\mathbf{r}, t)=b_0+b_1(\mathbf{r}, t)$ to the fluctuations of the distribution function. Equations (5), (8), and (9) give a complete description of a uncharged HFC.

We now extend the transport equation (5) to the case of a charged system. Let $\mathbf{E}(\mathbf{r},t)$ be a macroscopic longitudinal electric field, equal to the sum of the fields produced by the external charges and the polarization field. We assume that the field acts on the conduction electrons and on the f electrons. We can then write the generalized Landau–Silin equation in the form

$$\partial N_1/\partial t+\{\nabla_{\mathbf{r}}N_1\nabla_{\mathbf{k}}\epsilon_0\}-\{\nabla_{\mathbf{k}}N_0\nabla_{\mathbf{r}}\epsilon_1\}+e\mathbf{E}\nabla_{\mathbf{k}}N_0-i[\epsilon_1,N_0]-i[\epsilon_0,N_1]=I(N_1), \quad (10)$$

Solving Eqs. (8)–(10) simultaneously makes it possible to determine the dielectric response in the HFC to a longitudinal electric field. We restrict the analysis to the case in which the collision frequency is much lower than the frequency ω of the electric field. In this limit the collision integral can be ignored. The kinetic equation (10) can then be solved exactly, and we find the matrix N_1 as a functional of ϵ_1.

Let the electric field be a periodic function in space and time:

$$\mathbf{E}(\mathbf{r},t)=\mathbf{E}(\mathbf{q},\omega)\exp(i\mathbf{qr}-i\omega t)+\text{c.c.}$$

Fourier transforming with respect to the coordinate r, and solving the temporal differential equation, we obtain

$$N_1(\mathbf{k},\mathbf{q},\omega)=i\int_{-\infty}^{0}dy\ \exp(-i\epsilon_-y-i\omega y)(\epsilon_1(\mathbf{k},\mathbf{q},\omega)N_+$$

$$-N_-\epsilon_1(\mathbf{k},\mathbf{q},\omega)+ie\mathbf{E}\nabla_{\mathbf{k}}N_0)\exp(i\epsilon_+y), \quad (11)$$

where we have written $\mathbf{E}=\mathbf{E}(\mathbf{q},\omega)$. In addition, we introduce the matrices

$$\epsilon_\pm=\epsilon_0(\mathbf{k})\pm\tfrac{1}{2}\mathbf{q}\nabla_{\mathbf{k}}\epsilon_0(\mathbf{k}), \quad N_\pm=N_0(\mathbf{k})\pm\tfrac{1}{2}\mathbf{q}\nabla_{\mathbf{k}}N_0(\mathbf{k}). \quad (12)$$

The solution (11) can be simplified somewhat by using the approximation $\epsilon_\pm\approx\epsilon_0(\mathbf{k}\pm 1/2\mathbf{q})$, $N_\pm\approx N_0(\mathbf{k}\pm 1/2\mathbf{q})$, which corresponds to dropping the terms of order $0(q^2)$. This approximation is adequate for solving problems in which the electric field varies in space sufficiently slowly. On the basis of this approximation the matrices $\epsilon_\pm$ and $N_\pm$ can be diagonalized simultaneously by means of the unitary transformation U: $\epsilon_0(\mathbf{k})=U_{\mathbf{k}}^{-1}E_{\mathbf{k}}U_{\mathbf{k}}$, $N_0(\mathbf{k})=U_{\mathbf{k}}^{-1}f_{\mathbf{k}}U_{\mathbf{k}}$. Here $E_{\mathbf{k}}$ and $f_{\mathbf{k}}$ are diagonal matrices

$$E_{\mathbf{k}}=\delta_{\alpha\beta}\begin{pmatrix}E_{1\mathbf{k}} & 0\\ 0 & E_{2\mathbf{k}}\end{pmatrix}, \quad f_{\mathbf{k}}=\delta_{\alpha\beta}\begin{pmatrix}f(E_{1\mathbf{k}}) & 0\\ 0 & f(E_{2\mathbf{k}})\end{pmatrix}, \quad (13)$$

where $E_{1\mathbf{k}}$ and $E_{2\mathbf{k}}$ are the lower and upper hybridized bands, respectively. Moreover, $f(x)=[\exp((x-\mu)/T)+1]^{-1}$. In what follows, we assume that the total number of conduction electrons and f electrons in a unit cell is less than 2. Therefore, the lower band $E_{1\mathbf{k}}$ is only partially filled. Expressions for these bands are presented in, for example, Ref. 2 . Finally, we obtain the following approximate solution of the kinetic equation (10):

$$N_1(\mathbf{k},\mathbf{q},\omega)=i\int_{-\infty}^{0}dyU_-^{-1}\exp(-iE_-y-i\omega y)[U_-\epsilon_1(\mathbf{k},\mathbf{q},\omega)U_+^{-1}f_+$$

$$-f_-U_-\epsilon_1(\mathbf{k},\mathbf{q},\omega)U_+^{-1}+ie\mathbf{E}U_-\nabla_{\mathbf{k}}N_0U_+^{-1}]\exp(iE_+y)U_+. \qquad (14)$$

The lower indices $\pm$ correspond to the wave vectors $\mathbf{k}\pm\mathbf{q}/2$. Unfortunately, the complete expression for all matrix elements N_1 is too complicated. We therefore give only the result for N_1^c:

$$N_1^c(\mathbf{k},\mathbf{q},\omega)=ie(\mathbf{E}\mathbf{v}_{\mathbf{k}})f'(E_{1k})\cos^2\theta_k(\mathbf{q}\mathbf{v}_{\mathbf{k}}-\omega)^{-1}-ie\omega(\mathbf{E}\mathbf{v}_{\mathbf{k}})f(E_{1k})$$

$$\times\sin^2\theta_k\sin(2\theta_k)b_0^{-1}(\Delta_k^2-\omega^2)^{-1}+\cos^2\theta_k\sin\theta_kf'(E_{1k})$$

$$\times[\epsilon_1^f\sin\theta_k-(b_1(\mathbf{q},\omega)+b_1^*(-\mathbf{q},-\omega))\cos\theta_k]\frac{\mathbf{q}\mathbf{v}_{\mathbf{k}}}{\mathbf{q}\mathbf{v}_{\mathbf{k}}-\omega}. \qquad (15)$$

Here the function θ_k is related to the band E_{1k} by the relation $E_{1k}=\epsilon_f-b_0\cot\theta_k$. The quantity $\Delta_k=E_{2k}-E_{1k}=2b_0/\sin(2\theta_k)$ is the direct gap between the hybridized bands. The quantity $\mathbf{v}_{\mathbf{k}}=\nabla_{\mathbf{k}}E_{1\mathbf{k}}=\mathbf{v}_{0\mathbf{k}}\cos^2\theta_{\mathbf{k}}$ is the velocity of the heavy quasiparticles in the band E_{1k}, and the quantity $\cos^2\theta_k=m_0/m^*$ describes the renormalization of the electron mass.

The first term in expression (15) corresponds to the change, standard for normal Fermi liquids, in the distribution function by the electric field **E**. The second term describes the change in the distribution function as a result of interband transitions. The last term describes the change in N_1^c produced as a result of the change in the interaction energy of the electrons due to a deviation from equilibrium.

For a complete solution of the problem it is necessary to find the change in the matrix of the quasiparticle energy (3) with the field **E** switched on. The matrix elements N_1^f and N_1^{cf} found from Eq. (14) must therefore be substituted into Eqs. (8) and (9) and the system of equations obtained must be solved.

Let us now consider the case of an almost static field: $0<\omega\leqslant qv_F$. Solving Eqs. (8) and (9) gives $\epsilon_1^f=-ie|\mathbf{E}|/q$, $b_1=0$. The function (15) is now completely determined. This makes it possible to find, using Eq. (7), the conductivity: $e\mathbf{J}(\mathbf{q},\omega)=\sigma(\mathbf{q},\omega)\mathbf{E}$. We thus obtain the following expression for the dielectric function in the limit $\omega\to0$:

$$\epsilon(q,0)=1+\frac{4\pi i\sigma(q,\omega)}{\omega}=\epsilon_0+\frac{q_s^2}{q^2}. \qquad (16)$$

Here $\epsilon_0=1+\omega_{pc}^2/6b_0^2$, the second term is the contribution of interband transitions to the polarization, and $\omega_{pc}^2=4\pi e^2N_c/m_0$ is the squared plasma frequency for noninteracting conduction electrons with concentration N_c and mass m_0. For the screening wave vector we have $q_s^2=4\pi e^2\rho_0$, where ρ_0 is the density of states in the band $\epsilon(\mathbf{k})$ at the Fermi surface, with allowance for the spin.

In the other important case — uniform alternating electric field ($q=0$) — the last term in Eq. (15) does not contribute to N_1^c. Calculating the conductivity $\sigma(0,\omega)$ first, we obtain for the dielectric function the expression

$$\epsilon(0,\omega)=1-\frac{4\pi e^2\rho_0 v_{0F}^2 m_0}{3\omega^2 m^*}+\frac{2\pi e^2}{3b}\sum_{k\leq k_F} v_{0k}^2\sin^3(2\theta_k)(\Delta_k^2-\omega^2)^{-1}, \tag{17}$$

which gives results that are in complete agreement with the microscopic theory of Ref. 7 for Anderson's lattice model. Specifically, the system under study is characterized by two plasma frequencies. The low plasma frequency is determined by the relation $\omega_p^2=6T_0^2$, i.e., it is of the order of the Kondo temperature T_0. The high plasma frequency is equal to the unrenormalized frequency ω_{pc}; i.e., in the region of rf oscillations the interaction of the conduction electrons with the f electrons is insignificant.

In conclusion, we note that the result (15) [or (16)] can be used to study other types of collective excitations, for example, spin waves. Including a magnetic field in Eq. (10) will also make it possible to investigate the galvanomagnetic properties of HFCs by the methods developed for normal metals.

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