Effect of magnetic field on the thermodynamic and kinetic properties of Kondo lattices at low temperatures

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The thermodynamic (heat capacity C, magnetic susceptibility χ) and kinetic (resistivity ρ, thermoelectric power S, thermal conductivity $\varkappa$, quantum absorption) properties of Kondo systems with heavy fermions in a magnetic field are investigated for the Coqblin–Schrieffer model in the $1/N$ expansion. The field dependences of $C(H)$ and $\chi(H)$ in the temperature range corresponding to a coherent state of the Kondo lattice agree with the experimental data. Qualitative agreement between the calculated kinetic properties under coherent conditions and the experimental data is obtained if account is taken of carrier scattering by normal impurities and Kondo bosons. The expressions obtained for $C(H,T)$, $\chi(H,T)$, $\rho(H,T)$, $S(H,T)$ and $\chi(H,T)$ confirm the anomalously strong dependence of the Kondo-lattice properties on the temperature and on the magnetic field strength in the coherent state, and the presence of a single energy scale T_0 of the order of the Kondo temperature.

INTRODUCTION

Research into systems with heavy fermions and variable valency have recently attracted much attention by both experimenters and theoreticians (see the reviews, Refs. 1–5). This interest is due to a number of anomalies in the properties of these substances, such as thermodynamic (heat capacity C), kinetic (resistivity ρ, thermoelectric power S, thermal conductivity $\varkappa$), magnetic (susceptibility χ), and others. The main cause of the onset of these properties is the Kondo effect, i.e., the interaction of conduction electrons with localized $4f$ (or $5f$) electrons. When the Kondo-impurity density is low, the scattering of the conduction electrons by each impurity can be regarded as independent. The properties of such systems have by now already been investigated in detail. If the Kondo-impurity density is high enough, the scattering processes can no longer be regarded as independent, and account must be taken of coherent-scattering effects. Of greatest interest are substances in which rare-earth atoms with localized $4f$ (or $5f$) electrons form a regular lattice. The low-temperature properties of such systems are determined by the onset of a coherent Kondo state characterized by the appearance of fermions with anomalously large effective masses on the Fermi surface. The properties of substances with heavy fermions differ greatly in many respects from those of substances with low Kondo-impurity density, and are more similar to the properties of normal metals, but with an anomalously low effective Fermi energy [$\varepsilon_F^* \sim T_K$ (the Kondo temperature)]. Owing to the anomalously low value of ε_F^*, the thermodynamic and kinetic properties of heavy-fermion systems have anomalously strong dependences on the temperature T and on the magnetic field H.

We consider in the present paper, in the framework of the $1/N$ expansion for the Coqblin–Schrieffer model (i.e., without allowance for the valency change), the effect of the magnetic field on the thermodynamic and kinetic properties of Kondo lattices in the region of the coherent state, i.e., at $T \ll T_K$. The thermodynamic properties of a Kondo lattice in a magnetic field are dealt with in the coherent regime in Sec. 1. Section 2 is devoted to carrier scattering due to interaction between conduction electrons and localized f electrons. The magnetoresistance of a Kondo lattice, with allowance for carrier scattering by normal impurities and by Kondo bosons, is considered in Sec. 3. The thermoelectric power, the thermal conductivity, and the quantum absorption in a Kondo lattice are investigated in Secs. 4–6. Some numerical estimates permitting comparison of our results with experimental data are given in the conclusion.

1. THE MODEL. THERMODYNAMIC PROPERTIES

We shall investigate the properties of compounds with heavy fermions in the Kondo limit, where it is is assumed that the f level is deep enough in the band (i.e., the temperature dependence and the valency fluctuations of the f atoms can be neglected), while the Hubbard-repulsion energy of the f electrons is high enough. In this case, using a canonical transformation,[6] the Anderson Hamiltonian with direct direct hybridization (V) of the c and f electrons is transformed into the effective Coqblin–Schrieffer Hamiltonian[6] with an exchange-interaction constant $J = V^2/E_f$ where E_f is the position of the f level relative to the Fermi level.

The Hamiltonian of the Coqblin–Schrieffer lattice model is

$$H = \sum_{\mathbf{k}m} \varepsilon_{\mathbf{k}} c_{\mathbf{k}m}^{+} c_{\mathbf{k}m} - \frac{|J|}{N} \sum_{mm'} \sum_{\alpha} c_{\alpha m}^{+} f_{\alpha m} f_{\alpha m'} c_{\alpha m'}, \qquad (1)$$

where $c_{\alpha m}^{+}$ and $c_{\alpha m}$ are the creation and annihilation operators of the conduction electrons on site α, with component m of the angular momentum j; $f_{\alpha m}^{+}$ and $f_{\alpha m}$ are the creation and annihilation operators of the localized f electrons. We assume total degeneracy $N = 2j + 1 \gg 1$, which justifies the $1/N$ expansion.[5] The number of f electrons on each N-fold degenerate level is fixed and equal to

$$\sum_{m} f_{\alpha m}^{+} f_{\alpha m} = q_0 N. \qquad (2)$$

The main idea that allows us to investigate the properties of a system with Hamiltonian (1) is that the Hubbard–Stratono-

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vich transformation can be used to eliminate the four-fermion term of (1). This transformation introduces Bose fields into the theory. For the model (1) they are sometimes called Kondo bosons,[7] while for models with variable valency their analogs are called "slave bosons."

To study the properties of the model (1) we use the $1/N$ expansion method developed for the case of one f impurity and generalized for the case of a Kondo lattice.[5,7-10] The partition function Z is represented by the functional integral

$$Z=\int D\prod_{\alpha,m} c^{*}cf^{*}f\lambda r\exp\left\{-\int_{0}^{\beta}d\tau\mathscr{L}(\tau)\right\}, \tag{3}$$

where $c^{*}_{\alpha m}, c_{\alpha m}, f^{*}_{\alpha m}, f_{\alpha m}$ are Grassmann variables, while λ_α and r_α are real Bose variables. The Lagrangian of the system in a magnetic field is

$$\begin{aligned}\mathscr{L}(\tau)=&\sum_{km}[c_{km}^{*}(\partial_\tau+\varepsilon_k+g\mu_B Hm-\mu)c_{km}\\&+f_{km}^{*}(\partial_\tau+g\mu_B Hm-\mu)f_{km}]\\&+\sum_{\alpha m}\left[\frac{1}{|J|}r_\alpha^{2}+(c_{\alpha m}^{*}f_{\alpha m}+\text{h. c.})r_\alpha+i\lambda_\alpha(f_{\alpha m}^{*}f_{\alpha m}-q_0)\right],\end{aligned} \tag{4}$$

where μ is the chemical potential.

The Bose variable $r_\alpha(\tau)$ appears when the Hubbard–Stratonovich transformation is applied to the four-fermion term in Hamiltonian (1). Integration with respect to the auxiliary variable $\lambda_\alpha(\tau)$ ensures satisfaction of the condition (2) on each site of the Kondo lattice.

The partition function (3) for $N\gg 1$ is calculated by the saddle-point method with integration over the variables r_α and λ_α. At the saddle point we have

$$r_\alpha(\tau)=r_0, \qquad i\lambda_\alpha(\tau)=\varepsilon_0, \tag{5}$$

where ε_0 determines the effective position of the f level while r_0 has the meaning of the effective hybridization parameter of the c and f electrons.

Using the canonical transformation

$$c_{km}=\sum_{\nu=1,2}u_{\nu k}a_{\nu km}, \quad f_{km}=\sum_{\nu}v_{\nu k}a_{\nu km},$$

$$u_{1k}=v_{2k}=\cos\alpha_k, \quad u_{2k}=-v_{1k}=\sin\alpha_k, \quad \operatorname{ctg}2\alpha_k=(\varepsilon_0-\varepsilon_k)/2r_0, \tag{6}$$

the Lagrangian (4) can be diagonalized in the mean-field approximation; it takes the form

$$\mathscr{L}_0(\tau)=\sum_{\nu mk}a_{\nu km}^{*}(\partial_\tau+E_{\nu km}-\mu)a_{\nu km}+N\sum_{\alpha}[r_0^{2}/|J|-\varepsilon_0 q_0], \tag{7}$$

where

$$E_{\nu km}={}^1\!/_2[\varepsilon_0+\varepsilon_k\mp((\varepsilon_0-\varepsilon_k)^2+4r_0^2)^{1/2}]+g\mu_B Hm \tag{8}$$

corresponds to two hybridized bands (the subscripts $\nu=1$ and $\nu=2$ label respectively a plus and minus sign). The band structure is shown schematically in Fig. 1.

The energies $E_{\nu km}$ can be represented, using (6), in the convenient form

$$E_{1km}=\varepsilon_0-r_0\operatorname{ctg}\alpha_k+g\mu_B Hm, \quad E_{2km}=\varepsilon_0+r_0\operatorname{tg}\alpha_k+g\mu_B Hm. \tag{9}$$

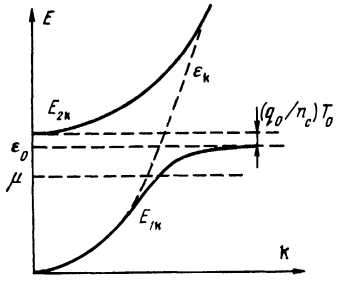

FIG. 1. Renormalized band structure of Kondo lattice in a coherent state.

The thermodynamic properties of the system in a magnetic field are determined by the dependences of the parameters ε_0 and r_0 on T and H, which should be determined by a self-consistent solution of the equations

$$\begin{aligned}&\frac{1}{N}\sum_{\nu km}\frac{\partial E_{\nu km}}{\partial\varepsilon_0}f(E_{\nu km})=q_0,\\&\frac{1}{N}\sum_{\nu km}\frac{\partial E_{\nu km}}{\partial r_0}f(E_{\nu km})=-\frac{2r_0}{|J|},\\&\frac{1}{N}\sum_{\nu km}f(E_{\nu km})=n_t=q_0+n_c,\end{aligned} \tag{10}$$

where $f(\varepsilon)=[\exp\{(\varepsilon-\mu)/T\}+1]^{-1}$, and Nn_c is the number of c electrons per Kondo-lattice site. We assume hereafter that the total number of c and f electrons ($n_t=g_0+n_c$) per orbital in each lattice site is less than unity. In this case, at zero temperature, the chemical potential μ is located in the lower band E_{1k} (see Fig. 1). The contribution of the upper band at sufficiently low temperatures ($T\ll T_K$) can therefore be neglected when considering both the thermodynamic and the kinetic properties. To solve the system (10) we assume that the nonrenormalized electron band ε_k is isotropic ($\varepsilon_k=\mathbf{k}^2/2m_0$), and the density of states near the Fermi surface does not depend on the energy ($\nu(\varepsilon)\approx\nu_0$). According to (9), the density of states in the lower renormalized band E_{1k} in a zero magnetic field is equal in these approximations to

$$\nu^{*}(E)=\sum_{k}\delta(E-E_{1k})=\nu_0\left(1+\frac{r_0^{2}}{(\varepsilon_0-E)^2}\right)=\frac{\nu_0}{\cos^2\alpha_{k(E)}}. \tag{11}$$

Analysis of the system (10) shows that a coherent state with $r_0\neq 0$ takes place at a temperature lower than T_K, which is determined from the first two equations of (10) as $r_0\to 0$:

$$\varepsilon_0(T)-\mu=T\ln[(1-q_0)/q_0],$$

$$\int_0^{2D}d\varepsilon\nu(\varepsilon)\frac{f(\varepsilon)-f(\varepsilon_0(T))}{\varepsilon_0(T)-\varepsilon}=\frac{1}{|J|},$$

where D is the half-width of the initial band. There is no known solution of this equation for arbitrary q_0. In the case $q_0\approx 1/2$ and $\nu_0|J|\ll 1$ we obtain for T_K

$$T_K\approx\alpha\frac{n_c}{\nu_0}\exp(-1/\nu_0|J|), \tag{12}$$

where $\alpha \approx 2e^C/\pi$ and C is the Euler constant.

At low temperatures $T \ll T_K$ the dependence of the parameters ε_0, r_0, μ, and of the renormalized density of states ν^* on the Fermi level on T takes at $H=0$ form

$$\begin{aligned} \tilde{\varepsilon}_0(T) &= \tilde{\varepsilon}_0(0)\,[1+(\pi^2/6)\,(T/T_0)^2], \quad \tilde{\varepsilon}_0 = \varepsilon_0 - \mu, \\ r_0(T) &= r_0(0)\,[1-(\pi^2/12)\,(T/T_0)^2], \\ \mu(T) &= \mu(0) + (\pi^2/6)\,(q_0/n_c)\,(T/T_0)^2 T_0, \\ \nu^*(T) &= \nu^*(0)\,[1-(\pi^2/2)\,(T/T_0)^2], \end{aligned} \tag{13}$$

where

$$T_0 \equiv \tilde{\varepsilon}_0(0) \approx (n_c/\nu_0)\exp(-1/\nu_0|J|),$$

$$r_0(0) = \left(\frac{q_0 T_0}{\nu_0}\right)^{1/2}, \quad \mu(0) = \frac{n_c}{\nu_0} - \frac{q_0}{n_c} T_0, \quad \nu^*(0) = \nu_0 + \frac{q_0}{T_0} \gg \nu_0. \tag{14}$$

It should be noted that the value of T_0 given by (14) agrees with the Kondo temperature only accurate to a numerical factor [see Eq. (12)]. This numerical factor depends on q_0 and on the form of the function $\nu(\varepsilon)$.

According to Eq. (9), the effective mass m^* on the Fermi surface in the hybridized band $E_{1\mathbf{k}}$ becomes at $H=T=0$ much larger than m_0:

$$m^*/m_0 = \cos^{-2}\alpha_{kF} = q_0/\nu_0 T_0 \gg 1.$$

A magnetic field has an anomalously strong influence on the parameters of the renormalized bands, and for $T=0$ we obtain

$$\begin{aligned} \varepsilon_0(H) &= \varepsilon_0(0)\,[1+{}^1/_6 j(j+1)\,(g\mu_B H/T_0)^2], \\ r_0(H) &= r_0(0)\,[1-{}^1/_{12} j(j+1)\,(g\mu_B H/T_0)^2], \\ \mu(H) &= \mu(0) + {}^1/_6 \pi^2 j(j+1)\,(g\mu_B H/T_0)^2 (q_0/n_c)\,T_0. \end{aligned} \tag{15}$$

The cause of the anomalously strong dependence on T and H is that T_0 for the known Kondo systems is of the order of several degrees or even of fractions of a degree.

Let us examine the effect of weak magnetic fields on the heat capacity C and on the magnetic susceptibility χ of a Kondo lattice:

$$C = \frac{1}{T}\sum_m \int d\varepsilon \nu^*(\varepsilon)\,(\varepsilon + g\mu_B H m - \mu)^2 \frac{df(\varepsilon')}{d\varepsilon'}\Big|_{\varepsilon' = \varepsilon + g\mu_B H m} \tag{16}$$

$$\chi = -g^2\mu_B{}^2 \sum_m m^2 \int d\varepsilon \nu^*(\varepsilon) \frac{df(\varepsilon')}{d\varepsilon'}\Big|_{\varepsilon' = \varepsilon + g\mu_B H m}. \tag{17}$$

As $T \to 0$ we obtain for the linear heat-capacity coefficient $\gamma(H) = C(H)/T$ and for the susceptibility, according to (16) and (17),

$$\gamma(H) = \frac{\pi^2}{3}\sum_m \nu^*(\mu - g\mu_B H m), \tag{18}$$

$$\chi(H) = g^2\mu_B{}^2 \sum_m m^2 \nu^*(\mu - g\mu_B H m). \tag{19}$$

In the lowest order in H, using (11) and (15), we obtain

$$\gamma(H) = \gamma(0)\,[1+{}^1/_2 j(j+1)\,(g\mu_B H/T_0)^2], \tag{20}$$

$$\chi(H) = \chi(0)\,[1+{}^1/_{10}(4j^2+4j-3)\,(g\mu_B H/T_0)^2], \tag{21}$$

where

$$\gamma(0) = {}^1/_3 \pi^2 N \nu^*(0),$$
$$\chi(0) = {}^1/_3 g^2 \mu_B{}^2 j(j+1)(2j+1)\nu^*(0).$$

An increase of $\gamma(H)$ in a magnetic field was obtained also in another model in Ref. 11. That result agreed with the experimental data for $\gamma(H)$ in $CeCu_2Si_2$ (Ref. 12). An increase of $\chi(H)$ in a magnetic field was observed, for example, in UPt_3 (Ref. 13) and $CeCu_2Si_2$ (Ref. 14).

If the magnetic field is increased the coherent state begins to break down, and for strong enough $H \geqslant H_c$ the parameter r_0 vanishes, corresponding to a transition to the incoherent Kondo-effect regime. The quantity H_c, generally speaking, is a function of temperature and can be obtained in principle from the condition that the system (10) be solvable. It is simplest to obtain H_c for $T=0$:

$$H_c = \frac{1}{N}\frac{e}{2^{1/N}}\left[\frac{(1-n_c)(1-q_0)}{n_c q_0}\right]^{q_0} \frac{1}{1-q_0} T_0. \tag{22}$$

One can expect the experimentally observed change of the field dependences of $\gamma(H)$ and $\chi(H)$, from an increase with increase of H to a decrease, is due to a transition from a coherent regime ($H < H_c$) to an incoherent one ($H > H_c$).

2. ELECTRON SCATTERING

To explain the kinetic properties of Kondo lattices in the coherent-state region, we investigate the effect of a magnetic field on the scattering of electrons by Kondo bosons.

We assume that the effect of the magnetic field on the electron scattering near the Fermi surface is determined mainly by the splitting, in the magnetic field, of the N-fold degenerate hybridized band $E_{1\mathbf{k}m}$. We neglect the effect of the magnetic field on the character of the electron motion near the Fermi surface. This approximation is justified because the magnetic field alters in the main the character of the motion of the conduction electrons (c-electrons), whereas the wave function of the electrons near the Fermi surface is composed mainly of f-electron wave functions, as follows from the canonical transformation (6), since $\cos^2\alpha_{kF} = m_0/m^* \ll 1$ on the Fermi surface.

Let us examine the fluctuations of the fields r and λ about their mean-field values:

$$\begin{aligned} r_\alpha(\tau) &= r_0 + \tilde{r}_\alpha(\tau) = r_0 + b_{1\alpha}(\tau), \\ i\lambda_\alpha(\tau) &= \varepsilon_0 + i\tilde{\lambda}_\alpha(\tau) = \varepsilon_0 + ib_{2\alpha}(\tau). \end{aligned} \tag{23}$$

Substituting (23) in (4) and using the transformations (6), we can represent the Lagrangian (4) in the form

$$\mathcal{L}(\tau) = \mathcal{L}_0(\tau) + \tilde{\mathcal{L}}(\tau), \tag{24}$$

where $\mathcal{L}_0(\tau)$ is given by Eq. (7) and

$$\tilde{\mathcal{L}}(\tau) = \sum_{r=1,2}\sum_{\mathbf{q}}\left[\frac{N}{2} g_r b_{r\mathbf{q}}{}^2(\tau) + b_{r\mathbf{q}}(\tau)\left(\sum_{\mu\nu}\sum_{mk} C_r{}^{\mu\nu}(\mathbf{k}, \mathbf{k}+\mathbf{q})\, a^+_{\nu\mathbf{k}+\mathbf{q}m}(\tau)\, a_{\mu\mathbf{k}m}(\tau) - d_r\delta_{\mathbf{q},0}\right)\right], \tag{25}$$

where

$$g_1 = 2/|J|, \quad g_2 = 0, \quad d_1 = -Nr_0/|J|, \quad d_2 = iq_0 N, \tag{26}$$

$$C_1{}^{\mu\nu}(\mathbf{k}, \mathbf{k}') = u_{\nu\mathbf{k}'} v_{\mu\mathbf{k}} + u_{\mu\mathbf{k}} v_{\nu\mathbf{k}'}, \quad C_2{}^{\mu\nu}(\mathbf{k}, \mathbf{k}') = i v_{\nu\mathbf{k}'} v_{\mu\mathbf{k}}. \tag{27}$$

Here μ and ν take on the values 1 and 2, while the functions $u_{\nu\mathbf{k}}$ and $v_{\nu\mathbf{k}}$ are defined by Eq. (6). To eliminate the divergences in the renormalization of the electron and boson Green's functions, we assume in the course of the calculations that $g_2 \neq 0$ and let g_2 go to zero in the final expressions. We find first of all the renormalized Green's function $b_{r\mathbf{q}}(\tau)$ of the boson field with allowance for the interaction with the electrons, in the leading order in the parameter $1/N$:

$$D_{rr'}(\mathbf{q}, i\omega_n) = \langle b_{r\mathbf{q}}(i\omega_n) b_{r', -\mathbf{q}}(-i\omega_n) \rangle, \tag{28}$$

where $\omega_n = 2\pi nT$ is the boson Matsubara frequency. In the leading order $O(1/N)$ the value of $\hat{D}$ is determined by the sum of the diagrams shown in Fig. 2, where the double (single) wavy line corresponds to the renormalized (unrenormalized) Green's function of the boson field:

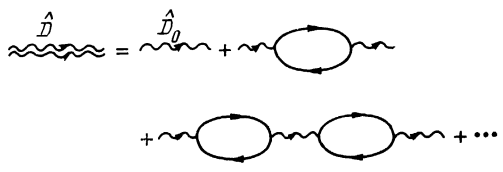

FIG. 2.

Each of the diagrams for $\hat{D}$ in this figure is of order $O(1/N)$. The summation yields the expression

$$\hat{D}(\mathbf{q}, i\omega_n) = \frac{1}{N}[\hat{\Pi}_0 - \hat{\Pi}(\mathbf{q}, i\omega_n)]^{-1}, \tag{29}$$

where

$$\hat{\Pi}_0 = \begin{pmatrix} g_1 & 0 \\ 0 & g_2 \end{pmatrix}, \tag{30}$$

$$\Pi_{rr'}(\mathbf{q}, i\omega_n) = -\frac{1}{N} \sum_{\mathbf{k}} \sum_{\nu\mu} \sum_{m} C_r^{\mu\nu}(\mathbf{k}, \mathbf{k}+\mathbf{q}) \times C_{r'}^{\nu\mu}(\mathbf{k}+q, k)[f(E_{\mu\mathbf{k}m}) - f(E_{\nu\mathbf{k}+\mathbf{q}m})][i\omega_n + E_{\mu\mathbf{k}m} - E_{\nu\mathbf{k}+\mathbf{q}m}]^{-1}. \tag{31}$$

Note that an investigation of the poles of the Green's function $\hat{D}$ can yield the spectrum of the Bose excitations.[15]

The renormalized Green's function of the electron is determined, in the leading order in $1/N$, by the sum of diagrams shown in Fig. 3, where the solid double (single) line corresponds to the renormalized (nonrenormalized) Green's function of the electron:

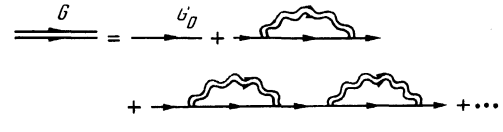

FIG. 3.

Since we are considering the case $n_t < 1$, scattering transitions of electrons from the lower band to the empty upper band can be neglected at low temperatures ($T \ll T_K$). The mass correction to the electron Green's function in the lower band takes in this case, in accordance with Fig. 3, the form

$$\Sigma_{1m}(\mathbf{k}, i\omega) = T \sum_{\omega_n} \sum_{\mathbf{q}} C_r^{11}(\mathbf{k}, \mathbf{k}+\mathbf{q}) C_{r'}^{11}(\mathbf{k}+\mathbf{q}, \mathbf{k}) \times [i\omega + i\omega_n - E_{1m\mathbf{k}+\mathbf{q}} + \mu]^{-1} D_{rr'}(\mathbf{q}, i\omega_n), \tag{32}$$

where $(\omega = 2\pi(n+1/2)T$ is the fermion Matsubara frequency.

The electron reciprocal lifetime in the lower band numbered m, with energy E, is determined by the imaginary part of the analytic contamination, in frequency, of the function $\Sigma(\mathbf{k}, i\omega)$ to the real axis:

$$\tau_m^{-1}(E) = -1/2 \operatorname{Im} \Sigma(E). \tag{33}$$

Since $\hat{D} \sim 1/N$, we have also $\Sigma \sim 1/N$, and consequently $\tau^{-1} \sim 1/N$. Cumbersome calculations, which we omit here, yield for electrons scattered by Kondo bosons near the Fermi surface

$$\tau_{Bm}^{-1}(E) = \frac{\pi}{8N} \frac{q_0}{n_t} \frac{(E-\mu)^2 + \pi^2 T^2}{T_0} \left[1 - 2\frac{g\mu_B Hm}{T_0} + 3\left(\frac{g\mu_B Hm}{T_0}\right)^2 + \frac{5}{6} j(j+1) \left(\frac{g\mu_B H}{T_0}\right)^2 \right]. \tag{34}$$

In this expression the last term is connected with the field dependence of the parameter $r_0(H)$ and $\varepsilon_0(H)$ [see (15)]. At $H = 0$ the result (34) agrees with the result of Ref. 16.

3. MAGNETORESISTANCE

For systems with independent Kondo impurities (low density of rare-earth atoms), a negative magnetoresistance is observed[1,13,14] and is due to the suppression of the Kondo effect by the magnetic field and to the corresponding decrease of the reciprocal lifetime τ^{-1} of the conduction electrons. The situation is reversed for Kondo lattices in the coherent state (i.e., in the $T < T_K$ region). At temperatures $T < T_K$ experiment yields a positive magnetoresistance.[13,14] A transition from negative to positive magnetoresistance when the temperature was lowered was observed in a number of compounds, for example in $CeAl_3$.[14] At $T \ll T_K$ the resistivity ρ depends on T and H as follows:

$$\rho(H) = \rho_0 + A(H) T^2. \tag{35}$$

The residual resistivity ρ_0 for systems with heavy fermions is of the same order as in a normal metal ($\rho_0^{-1} = e^2 N \nu_0 v_{F0}^2 \tau_0/6$) for scattering by impurities.[17,18] It can be shown that, notwithstanding the strong temperature and field dependences of the density of states [see Eqs. (11), (13), and (15)], the resistivity due to scattering by impurities does not depend on T or H. In a zero magnetic field, the presence of the term AT^2 in $\rho(H = 0)$ is due to scattering by Kondo bosons.[7,16,19] Turning on a magnetic field increases the coefficient A, as observed in experiment for various Kondo systems such as $CeCu_2Si_2$, $CeAl_3$, UBe_{13} (Ref. 14) and UPt_3 (Ref. 13).

Within the framework of standard kinetics, we introduce for the calculation of various kinetic coefficients the following quantities:

$$L_m^{(n)} = \frac{N}{3} \int dE \nu^*(E) v^{*2}(E) \left(-\frac{\partial f(E_m)}{\partial E_m} \right) (E_m - \mu)^n \tau_m(E_m), \tag{36}$$

where $E_m = E + g\mu_B Hm$, the density of states $\nu^*(E)$ is defined in (11), and the electron velocity $v^*(E)$ in the renormalized band is of the form

$$v^{*2}(E)=\left|\frac{\partial E_{1\mathbf{km}}}{\partial \mathbf{k}}\right|_{E_{1\mathbf{km}}=E}=\frac{2}{m_0}\left(E+\frac{r_0^2}{\varepsilon_0-E}\right)\cos^{-4}\alpha(E). \quad (37)$$

In the calculation of the kinetic coefficients at low temperatures it is necessary to take into account, besides scattering by Kondo bosons, also scattering by normal impurities. Regarding these impurities as pointlike, we easily obtain for the reciprocal relaxation time the known result[17,18]:

$$\tau_{imp,m}^{-1}(E)=\tau_0^{-1}\cos^2\alpha(E-g\mu_B Hm), \quad (38)$$

where τ_0^{-1} is the reciprocal lifetime in the normal metal for scattering by pointlike impurities. The total lifetime contained in (36) is given by

$$\tau_m^{-1}(E)=\tau_{imp,m}^{-1}(E)+\tau_{Bm}^{-1}(E). \quad (39)$$

Using (36), we can represent the conductance in the form

$$\sigma=e^2\sum_m L_m^{(0)}. \quad (40)$$

Assuming that $\tau_{\text{imp}}^{-1}\gg\tau_B^{-1}$, at low temperatures, we obtain for the coefficient $A(H)$ in expression (35) for the resistance

$$A(H)=A(0)[1+{}^{11}/_{3}j(j+1)(g\mu_B H/T_0)^2], \quad (41)$$

$$A(0)=\frac{\pi^4}{4N^2}\left(\frac{q_0}{n_t}\right)^2\frac{h}{e^2k_F}\frac{1}{T_0^2}, \quad (42)$$

where $\hbar k_F$ is the momentum on the Fermi surface. Expression (42) agrees with the results of Refs. 7, 16, and 19. Here and henceforth we put $q_0\ll n_c$; this does not change qualitatively the character of the dependences of the coefficients on H, but simplifies the expressions substantially.

Note that for ordinary electron–electron collisions Eq. (42) contains in place of T_0 the Fermi energy $\varepsilon_F\gg T_0$. As seen from (41), in the low-temperature coherent state compounds with heavy fermions have an anomalously large positive magnetoresistance. The experimentally observed[13,14] $A(H)$ dependence is in good qualitative agreement with (41).

4. THERMOELECTRIC POWER

We consider the behavior of the thermoelectric power as a function of temperature and magnetic field in the region of the coherent state ($T\ll T_K$). Using the coefficients (36), we can express the thermoelectric power S in the form

$$S=-\frac{1}{eT}\left(\sum_m L_m^{(1)}\right)\Big/\sum_m L_m^{(0)}. \quad (43)$$

Assume that at the very lowest temperatures the carriers are scattered mainly by normal impurities ($\tau_{\text{imp}}^{-1}\gg\tau_B^{-1}$). Using (38) and (43) we obtain then

$$S_{imp}(T,H)=S_{imp}(T,0)[1+{}^{1}/_{2}j(j+1)(g\mu_B H/T_0)^2], \quad (44)$$

$$S_{imp}(T,0)=-\frac{\pi_2}{3}\frac{k_B}{|e|}\frac{T}{T_0}. \quad (45)$$

Thus, in the impurity scattering region, the thermoelectric power of a Kondo lattice has a negative sign (just as for a normal metal, in which the carriers are electrons) and an anomalously large value. The reason for the large thermoelectric power is that (45) contains the ratio $T/\tilde{\varepsilon}_0$ and not T/ε_F as in a normal metal. As seen from (44), turning on a magnetic field leads to the appearance of anomalously large positive field corrections.

The situation is entirely different when scattering by Kondo bosons predominates. Using (34) and (43) we get

$$S_B(T,H)=S_B(T,0)[1-{}^{7}/_{6}j(j+1)(g\mu_B H/T_0)^2], \quad (46)$$

$$S_B(T,0)=2\frac{k_B}{|e|}\frac{\pi^2(21-\pi^2)}{\pi^2+3}\frac{T}{T_0}. \quad (47)$$

In this case the thermoelectric power is positive and is decreased by turning on the magnetic field.

Analysis of expression (43) at $\tau^{-1}=\tau_B^{-1}+\tau_{\text{imp}}^{-1}$ shows that the thermoelectric power should reverse sign at a temperature

$$T_s=\frac{T_0}{(\mu\tau)^{1/2}}\left(\frac{4Nn_c}{\pi^3 q_0}\right)^{1/2}. \quad (48)$$

Since the parameter $\mu\tau_0$ can be very large, depending on the purity of the sample (recall that τ_0 is the time of electron relaxation on normal impurities in a nonrenormalized band), we can expect to get $T_s\ll T_0\sim T_K$. At temperatures $T<T_S$ the thermoelectric power is negative and is given by (44). For $T>T_S$ the thermoelectric power is positive and takes the form (46). A qualitative plot of the thermoelectric power versus temperature is shown in Fig. 4. Note that the characteristic value of the temperature T_S at which the thermoelectric power reverses sign (this corresponds to a transition from one scattering mechanism to another) can differ substantially from the temperature T_ρ at which scattering by Kondo bosons makes the resistivity of the same order as the residual resistivity. Estimates show that

$$T_\rho/T_s\sim(n_c/q_0)^{1/2}. \quad (49)$$

This value can be much larger than unity in the model considered. Thus, the experimental observation of a positive magnetoresistance, which agrees with our result (41) for the principal mechanism of scattering by normal impurities, and the positive thermoelectric power observed in a number of experiments[13,1] in the same temperature interval, do not contradict the results (44) and (47). We found no experimental data on the thermoelectric power at the very lowest temperatures, where a negative thermoelectric power could be expected.

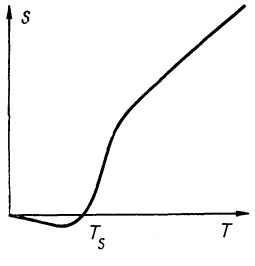

FIG. 4. Qualitative dependence of the thermoelectric power of a Kondo lattice in a coherent state ($T\ll T_K$). The reversal of the sign of the thermoelectric power at the point T_S is due to enhancement of the carrier scattering by Kondo bosons. Note that, nevertheless, the main contribution to the resistivity in the very same temperature region is made by scattering on normal impurities.

5. THERMAL CONDUCTIVITY

Using the coefficients (36), the electron contribution to the thermal conductivity $\varkappa$, and the Lorentz number $\mathscr{L}$ can be written in the form

$$\varkappa=\frac{1}{T}\left[\left(\sum_m L_m^{(2)}\right)-\left(\sum_m L_m^{(1)}\right)^2\Big/\sum_m L_m^{(0)}\right], \quad (50)$$

$$\mathscr{L}=\varkappa/\sigma T. \quad (51)$$

In this temperature region, where the carriers are scattered mainly by normal impurities, we can obtain by using (38), (50), and (51)

$$\varkappa_{imp}(T, H)=T\mathscr{L}_{imp}/\rho_0, \quad (52)$$

where ρ_0 is the residual resistivity defined in Sec. 3, and $\mathscr{L}_{imp}$ is the Lorentz number, which takes in our case the form

$$\mathscr{L}_{imp}=\mathscr{L}_0\left[1-\frac{\pi^2}{3}\frac{q_0^2}{n_t^2}\left(\frac{T}{T_0}\right)^2\left(1+j(j+1)\left(\frac{g\mu_B H}{T_0}\right)^2\right)\right], \quad (53)$$

$$\mathscr{L}_0=^1/_3\pi^2k_B^2/e^2. \quad (54)$$

With increase of temperature, carrier scattering by Kondo bosons becomes significant. In the temperature interval in which the principal mechanism is scattering by bosons, we can obtain by using (34), (50), and (51), in the lowest order in the temperature,

$$\varkappa_B(T, H)=T\mathscr{L}_B/\rho_B, \quad (55)$$

$$\mathscr{L}_B=\mathscr{L}_0\frac{21-\pi^2}{1+\pi^2/3}\approx 2.6\mathscr{L}_0. \quad (56)$$

It is seen from (52) that at the very lowest temperatures, the thermal conductivity in scattering by normal impurities is proportional to the temperature. As the temperature rises and the role of scattering by bosons increases, the character of the temperature dependence should change. Since $\rho_B \propto T^2$, in the region where scattering by bosons predominates the thermal conductivity is inversely proportional to the temperature. A qualitative plot of the electron contribution to the thermal conductivity of a Kondo lattice in the temperature region corresponding to the coherent state is shown in Fig. 5(a). This plot agrees with experiment.[13] Figure 5(b) shows the qualitative temperature dependence of the quantity $\mathscr{L}/\mathscr{L}_0$. At the very lowest temperatures we have $\mathscr{L}/\mathscr{L}_0<1$ (impurity scattering). As the temperature rises and the role of the Kondo bosons increases, the ratio $\mathscr{L}/\mathscr{L}_0$ becomes large than unity and reaches $\mathscr{L}/\mathscr{L}_0\approx 2.6$ at $T\ll T_0$. This character of the Lorentz-ratio temperature dependence agrees with the experimental observation.[13]

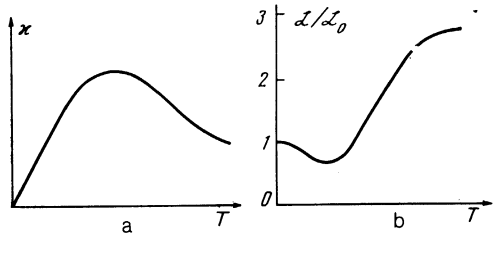

FIG. 5. Schematic temperature dependences: a—of the thermal conductivity (in the impurity-scattering region $\varkappa \propto T$, and when the role of the kondo bosons increases the dependence is reversed, $\varkappa \propto T^{-1}$); b—of the value of $\mathscr{L}/\mathscr{L}_0$ (in the region of impurity scattering the value $\mathscr{L}=\varkappa/\sigma T$ is less than the Lorentz number $\mathscr{L}_0=\pi^2k_B^2/3e^2$, as against $\mathscr{L}/\mathscr{L}_0\approx 2.6$ in the region of scattering by Kondo bosons).

6. QUANTUM ABSORPTION

The onset of two hybridized bands at $T<T_K$ should lead to the onset of quantum absorption due to interband electron transitions. Absorption of electromagnetic waves (without allowance for processes in which phonons participate) sets in at frequencies

$$\omega\geqslant\omega_0=2r_0=2T_K[(m^*/m_0)-1]^{1/2}. \quad (57)$$

The considered quantum electronic transitions between two hybridized bands leads to an additional contribution to the optical conductivity. Calculation of this contribution at $T=0$ yields

$$\sigma_{im}(\omega)=\frac{\pi e^2Nn_t}{4m_0}\left(\frac{\omega_0}{\omega}\right)^2(\omega^2-\omega_0^2)^{-1/2}. \quad (58)$$

As seen from (58), the contribution of direct electronic transitions between hybridized bands to the optical conductivity of Kondo lattices has a characteristic threshold at the frequency $\omega=\omega_0$. This threshold singularity "shuts off" when account is taken both of the finite lifetime of the electrons and of the temperature. Notice must also be taken of the strong dependence of the contribution (58) on the magnetic field, which follows from the dependence of r_0 on H [see Eq. (15)].

In addition to the direct interband transitions considered above, other indirect electron transitions with participation of phonons are present and contribute additionally to the optical conductivity, starting with energies $\hbar\omega$ on the order of the difference between the bottom E_{2k} of the upper band and the Fermi level, i.e., on the order of the energy $\Delta E=(r_0^2/\mu)+\tilde{\varepsilon}_0$, which equals at $T=0$ to T_0n_t/n_c, as follows from Eqs. (8) and (14). The contribution of indirect transitions should also depend strongly on T and H.

CONCLUSION

Our results show that the dependence on the thermodynamic and kinetic coefficients of the Kondo lattices in the coherent-state region on the magnetic field contains the same single energy parameter $T_0=q_0(m_0/m^*)/v_0$ as in the case of a zero magnetic field. Recall that in a normal metal such an energy parameter is the Fermi energy $\varepsilon_F\gg T_0$. The parameter T_0 for UPt_3 lies in the interval 20–30 K according to Ref. 2 and 27–48 K according to Ref. 13. The experimental data of Ref. 13 for UPt_3 yield estimates

$$a=^1/_{10}(4j^2+4j-3)(g\mu_B/T_0)^2,$$
$$b=^{11}/_{3j}(j+1)(g\mu_B/T_0)^2, \quad (59)$$

for the coefficients of H^2 expression (21) for the susceptibility χ and expression (41) for the resistivity ρ. According to Ref. 13, $a=1.35\times10^{-3}T^{-2}$ and $b=3.08\times10^{-3}T^{-2}$. Substituting in (59) the values $g=2.6$ (Ref. 13) and $j=5/2$, we obtain for $T_0=30$ K the values $a=1.24\times10^{-3}T^{-2}$ and $b=12.4\times10^{-3}T^{-2}$. Thus, the coefficient a obtained on the

basis of (21) and (59) agrees well with the observed $\chi(H)$ dependence, whereas the coefficient b, calculated from (41) and (59), deviates from the experimental value by approximately 4 times.

In conclusion, we note once more that a comparison of the theoretical results with experiment shows that the use of the $1/N$ expansion (even in lowest-order perturbation theory) leads to a correct qualitative and a satisfactory quantitative description of various anomalous properties of compounds with heavy fermions. We have considered, in a unified approach, the thermodynamic (C,χ) and kinetic $(\rho,S,\varkappa)$ properties of such compounds. The possible use of the $1/N$ expansion, however, is not restricted to the properties considered above. It is possible to investigate similarly other phenomena, such as ultrasound absorption, the Hall effect, and others.

Heavy-fermion compounds undergoing a magnetic or superconducting phase transitions at low temperatures are extensively investigated at present. Our results have a bearing on this rather large class of compounds, where such transitions are not observed or occur at a temperature lower than that of the transition to a coherent Kondo state.

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