Quantum tunneling in a metal and the heavy-electron problem

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If the spectrum of one-electron states in a metal has a relatively narrow density-of-states peak due to the presence of a narrow band, of hybridization, or in general of any phase region with low group velocity, then the electron polaron effect (EPE) [Yu. Kagan and N. V. Prokof 'ev, Sov. Phys. JETP **63**, 1276 (1986)] leads to a drastic decrease of the width of this peak. This narrowing is due to Coulomb interaction between the electrons in the density peak and the electrons in the remaining part of the phase space, and is pronounced stronger the less the one-particle value of the width and the stronger the effective interaction. If the renormalized width becomes smaller than the Debye temperature, an additional narrowing of purely phonon origin appears and is found to be nonlinearly amplified by the EPE. It becomes possible to explain the existence, in metals with transition elements, of heavy electrons with itinerant-motion energy scales on the order of 100 K or 10 K. At lower temperatures the coherent width decreases exponentially with T and incoherent motion sets in under disrupted-band conditions. Analysis of the heat capacity, of the magnetic susceptibility, and of the resistance agree qualitatively with the experimental behavior of these quantities as functions of T. At high temperatures the physical properties of the system have a power-law behavior with an exponent that depends on the interaction.

1. INTRODUCTION

1. We have reported in a preceding paper[1] a detailed analysis of the nature of the electron polaron effect (EPE) produced when a heavy (compared with the electron) particle moves in a metal. The EPE is produced because the many-electron wave function modified by the interaction with the particle contains a component that does not follow the moving particle adiabatically. This part of the wave function is due to virtual electron-hole pairs whose energy is lower than the characteristic energy ω of the motion of the heavy particles. In fact, the energy of these pairs is bounded from below by the reciprocal lifetime of the particle in the unit cell τ^{-1} (we use here and below $\hbar = 1$)—states with pairs of lower energy have no time to be formed before the particle leaves the cell. The projection of the nonadiabatic part of the many-electron wave function formed during the time of stay of the particle in the unit cell on the corresponding state in a neighboring cell is what produces the EPE. At low temperature T, the EPE leads to a strong decrease of the amplitude of the tunneling transition from cell to cell. This is due to the presence, in the restructured many-particle electron function of the metal, of a large number of low-energy electron-hole pairs which are known to be responsible for the so-called "orthogonality catastrophe" in the static case,[2,3] and for the infrared divergence[4] in transitions. The first ideas concerning the role of the "orthogonality catastrophe" in the problem of diffusion of a heavy particle in a metal were advanced by Kondo,[5] whose results were later summarized in a review paper.[6]

EPE causes a drastic narrowing of the band. The scale of this narrowing depends substantially on the cutoff of the infrared divergence at low frequency. This cutoff is due to the finite lifetime of the particle in the unit cell[7]:

$$\tilde{\Delta}_{coh} = \Delta \exp\left\{ - b \ln\left(\frac{\omega}{\pi T} \operatorname{sh} \pi T \tau \right) \right\}. \tag{1.1}$$

Here Δ is the width of the band in the absence of the polaron effect;

$$b = 2\rho^2(\varepsilon_F) \overline{|V(\mathbf{k}-\mathbf{k}')|^2 (1-\cos(\mathbf{k}-\mathbf{k}')\mathbf{g})}, \tag{1.2}$$

where $V(\boldsymbol{\kappa})$ is the Fourier component of the particle interaction with the electrons (with allowance for screening); the averaging is over the directions of the vectors $\mathbf{k}$ and $\mathbf{k}'$ on the Fermi surface; $\mathbf{g}$ is the displacement of the particle in the transition. Expression (1.2) corresponds to the Born approximation.

As $T \to 0$ the parameter τ is determined by the coherent character of the motion between the wells, and is equal to

$$\tau^{-1} = \gamma \tilde{\Delta}_{coh}. \tag{1.3}$$

The width of the band is then

$$\tilde{\Delta}_{coh}(T=0) = \Delta_* = \Delta (\gamma\Delta/\omega)^{b/(1-b)}. \tag{1.4}$$

In the region $T \ll \Delta$ there is pure itinerant motion with scattering by the electrons that do not participate in the formation of the EPE. At $\Omega_T > \gamma\Delta$. Where

$$\Omega_T = 2\pi b T, \tag{1.5}$$

Δ_{coh} (1.1) decreases exponentially with rise of temperature. What is decisive then are transitions with excitation of the electronic subsystem. For these transitions the effective tunneling amplitude of the transition of the particles between the neighboring equivalent wells is equal to[1]

$$\tilde{\Delta}_0 = \Delta_0 \exp\{-b \ln(\omega/\pi T)\}. \tag{1.6}$$

The reflective fluctuations of the levels in neighboring cells, which are determined by Ω_T, despite the increase of $\Delta_0(T)$ (1.6), slow down the tunneling which progresses continuously with increase of T. This result reflects a phenomenon

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common to all problems of tunneling in a crystal, called "dynamic disruption" of the band.[9,8] The result is a regime of diffusion that slows down with the increase of T, and an ever increasing quasilocalization of the particle in the cell.

2. Once the physical nature of the EPE is understood, it is logical to conclude that a similar polaron effect should be experienced[5] not only by heavy particles, but also by any group of electrons near the Fermi surface, having a group velocity v_g that is small compared with the velocity of the electrons in the remaining part of phase space. Indeed, in this case the reciprocal time of stay of the electron in the unit cell is

$$\tau^{-1}\sim v_g/a\ll\varepsilon_0, \tag{1.7}$$

where ε_0 is a characteristic scale of the electron energy, of the order of ε_F or of the width of the band. The characteristic frequency of the electron motion inside the unit cell and in the tunneling transition (in imaginary time) has naturally the same scale ε_0. This means that the nonadiabatic energy interval spans practically the entire spectrum and, at the logarithmic accuracy with which expressions (1.1) and (1.4) were obtained, ω should be replaced by ε_0. As a result, the Coulomb interaction of this group of electrons with the remaining electrons leads to a polaron effect that causes further decrease of v_g and smoothing of the spectrum; the latter is more drastic the stronger the initial inequality (1.7).

The entire picture is particularly clear when a narrow and broad band cross a Fermi level located inside the narrow band. The EPE leads inevitably to an additional strong narrowing of the narrow band, at a rate that depends on the ratio Δ/ε_0 in (1.4), i.e., on the bare relation between the band widths.

If the EPE causes τ^{-1} to become smaller than the characteristic frequencies Θ_D of the phonon spectrum, the ordinary phonon polaron effect (PPE) due to the overlap of the phonon wave functions upon localization of the electrons in neighboring cells will set in simultaneously. The two polaron effects are realized independently, and $\Delta_0(\Delta)$ in (1.1) and (1.4) should be taken to mean in this case

$$\Delta_0(\Delta)\to f\Delta_0(\Delta),\quad f=\begin{cases} e^{-\Phi}, & \Theta_D\tau>1\\ 1, & \Theta_D\tau\ll 1\end{cases}, \tag{1.8}$$

where Φ is the usual phonon polaron exponent which remains finite as $T\to 0$ in a three-dimensional crystal.

It is interesting that the EPE, as follows from (1.4), enhances the role of the PPE, since $\Delta_*\sim f^{1/(1-b)}$.

Although the parameter b does not exceed $\frac{1}{2}$ (the unitary limit), its value is usually comparable with this limit. It can therefore be assumed that the narrow one-frequency band will always undergo an additional strong narrowing by the EPE.

The foregoing results remain qualitatively in force also when the spectrum of the one-particle electronic states has a density-of-states peak due to hybridization of the f or d levels of the ions, which make up the regular crystal, with the wide-band electrons. Let the Hamiltonian term responsible for the hybridization be of the standard form.

$$\hat{H}'=\sum_{\mathbf{k}\sigma l}[v(\mathbf{k})\exp(-i\mathbf{k}\mathbf{R}_l)\hat{c}_{\mathbf{k}\sigma}^{+}\hat{f}_{l\sigma}+\text{h.c.}]. \tag{1.9}$$

If $v\ll\varepsilon_0$, the time of stay of an electron in a quasilocalized state at a site is sufficient for a polarization "jacket" of electron-hole pairs of the wide band to be formed via the electron-electron interaction. In the band $\mathbf{k}$ state, however, there is no such polarization effect in practice. (Arguments favoring the appearance of a polaron effect in this case were discussed for the limit $T=0$ in Ref. 10). Adhering to the premise of one-electron interactions in hybridization at low T, we should take v in (1.9) to mean a transition amplitude that is diagonal in the occupation numbers of the electrons (and phonons). This leads to a many-electron wave-function overlap integral that has the same structure as in the normal EPE. As a result, the bare vertex in (1.9) should be replaced in analogy with (1.1) by

$$\tilde{v}_{coh}=v\exp\left\{-b'\ln\left(\frac{\varepsilon_0}{\pi T}\operatorname{sh}\pi T\tau\right)\right\}, \tag{1.10}$$

where b' differs from b (1.2) by the replacement $1-\cos(\mathbf{k}-\mathbf{k}')g\to 1/2$. Allowance for the PPE requires a replacement similar to (1.8) for v. This leads to a narrowing of the effective-hybridization energy interval and to further flattening of the spectrum in this region. Hybridization leads to the appearance of a density-of-states peak whose width is now of the order of $\tilde{\Gamma}_{\text{coh}}\sim v_{\text{coh}}^2/\varepsilon_0$, with the total number of the states in the peak conserved. Recognizing that $\tau^{-1}\approx\tilde{\Gamma}_{\text{coh}}$ in this case (see below) we obtain from (10) in the limit as $T\to 0$

$$\Gamma_*\approx\Gamma(\Gamma/\varepsilon_0)^{2b'/(1-2b')}, \tag{1.11}$$

where Γ is the width of the peak in the absence of the EPE. The situation is thus similar to the narrowing of the narrow band in the two-well model.

One more remark is in order here. We have neglected in (10) the change produced in the hybridization matrix element by the restructuring of the electronic state produced by the transition near the Fermi surface (see Ref. 4 for details). In our case the transition from the $d(f)$ state to the continuum causes the decisive role in this restructuring to be assumed by scattering from an ion with orbital angular momentum $l=2(3)$. We assume the corresponding scattering phase shift to be small. We note also that although the hybridization matrix element undoubtedly depends on k, it enters in all the final results only in the form $|v^2|$ averaged over the angles. Thus allows us, without loss of generality, to put $v=\text{const}$ in (1.9).

Thus, *if within the framework of the one-electron problem there exists an energy density-of-states peak in an interval noticeably smaller than ε_0, due to the presence of a narrow band, to hybridization, or in general of a group of electrons with low group velocity, then the interelectron interaction leads inevitably to a substantial narrowing of the peak by the electron polaron effect, and this narrowing can be enhanced under certain conditions by the* PPE. If the Fermi level is located inside the initial one-particle peak of states, it remains inside also after a narrowing of arbitrary scale. (A possible exception is the case when the bare density peak contained an anomalously small number of electrons.) It is important that the narrowing does not presuppose a special position of ε_F relative to the fine structure of the one-particle spectral density or a rigidly determined number of electrons in the narrow band per atom of the transition ion. In this sense, the narrowing has a universal character.

Note that in the general case the converse is also valid: if

experiment reveals an anomalously narrow peak of the density of states in a metal near the Fermi level, part of the narrowing of this peak must be due to the EPE.

The scale of the narrowing, as follows from (1.4), (1.8), and (1.11) can be very appreciable, especially if b and b' are close to their limiting values $\frac{1}{2}$ and $\frac{1}{4}$, respectively. At a sufficiently low value of the bare ratios Δ/ε_0 or v/ε_0 the true width of the band or of the density peak readily reaches values of the order of hundreds or even tens of degrees while the one-particle values of Δ and Γ can be larger by one or even two orders of magnitude. It seems that the peculiarities of the behavior of many metallic compounds of rare-earth elements and actinides (see, e.g., the review by Lawrence *et al.*[11]) can be caused by the onset of narrow density-of-state peaks due to the EPE. This can pertain, in particular, to what are customarily called heavy-fermion systems, a feature of which is the appearance of an energy scale quite unusual for metals, on the order of tens of degrees (see, e.g., the reviews of Stewart *et al.*[12] and Lee *et al.*[13]). A similar statement can be made also with respect to many metallic systems containing elements with unfilled d shells. Thus, in the context of the developed premises one can understand the nature of the anomalies properties of A-15 compounds, whose explanation calls for a density-of-states peak of width on the order of hundreds of degrees with ε_F located within this peak, whereas all the one-electron calculation yield much larger energy scales (see, e.g., the revies of Testardi[14] and of Veger and Goldberg[15]). It is in fact the universality of this scale, as also on the whole of the properties of a large number of members of this family of compounds, which had remained the stumbling block for all theoretical models (see the article by Gor'kov,[16] written as a postscript to the translation of the Refs. 14 and 15).

It must be noted that the idea that the existence of an ultranarrow band or an ultranarrow peak of the density near ε_F could explain the anomalous properties of all these compounds is prevalent in the literature explicitly or implicitly. We cite in this connection the article by Overhauser and Appel[17] in the case of heavy fermions and the article by Aleksandrov *et al.*[18] The latter is remarkable in that it advances the idea that the narrow peak in the density of states of A-15 compounds can be due to the phonon polaron effect. It seems however, that the PPE by itself cannot ensure the required narrowing in these compounds.

3. A distinctive feature of the narrowed band produced by the EPE is that its width varies with temperature and that the character of the motion changes with increase of T. At $\Omega_T < \gamma\Delta_*(\Gamma_*)$ we have Fermi-liquid motion of electrons with a heavy effective mass $m_*/m_0 \sim \varepsilon_0/\Delta_*(\Gamma_*)$. But at $\Omega_T > \gamma\Delta_*(\Gamma_*)$ there is already dynamic disruption of the band and a transition to a diffusion that slows down with increase of T, and a tendency to quasilocalization and to appearance of independent (spin-carrying) scatterers. A continuous transition is realized here in natural fashion from a coherent pattern to an incoherent one, which the authors of Ref. 13 regard, for example, as the principal feature of heavy-fermion systems. The fact that at $T > \Delta_*(\Gamma_*)$ the light electrons "see" the heavy ones as quasilocalized, and furthermore randomly arranged (with $\nu < 1$ electrons per transition ion) is the reason why the resistivity assumes already at $T \lesssim \Delta_*(\Gamma_*)$ a value of the order of the maximum one with a subsequent relatively weak dependence on T (see Sec. 5). The distinctive character of the motion in the incoherent region is due to the nontrivial law of decrease of the specific heat with T in this region (see Sec. 3). In all cases, the power-law dependences of the physical quantities T are governed by the interelectron interaction (via b and b').

Note that the anomalous narrowing and the large effective mass are due in final analysis to electron-electron interaction, but only with that part of the interaction which is connected with the interaction of electron groups that differ in their kinematic properties that determine the EPE. The remainder of the interaction, particularly the interelectron interaction in the narrow band (under the assumption that $\nu < 1$) can be regarded as weak or, at any rate, indecisive. In this sense, the model considered is an alternative of models extensively discussed in connection with heavy fermions, with an almost-localized Fermi liquid, and with the Kondo lattice; these models require, in particular that ν be close to 1 (see Ref. 13 and the literature cited there). Moreover, our model pertains to all systems with $m_*/m_0 \gg 1$ and is in no way connected with that extremely large value of this ratio, which is used to distinguish formally heavy-fermion systems (see Ref. 12).

2. INITIAL RELATIONS

We write the system Hamiltonian for a narrow band intersecting with a wide one in the form

$$\hat{H} = \hat{H}_0 + \hat{H}'. \tag{2.1}$$

Here

$$\hat{H}_0 = \hat{H}_H + \hat{H}_L + \hat{H}_{HL} \tag{2.2}$$

is the Hamiltonian in the absence of tunneling transitions of heavy electrons (the subscripts H and L label the heavy and light electrons):

$$\hat{H}_L = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^{+} \hat{c}_{\mathbf{k}\sigma}, \qquad \hat{H}_H = \sum_{\mathbf{l}\sigma} \varepsilon_1 \hat{\nu}_{\mathbf{l}\sigma} + U_{HH}, \tag{2.3}$$

$$\hat{H}_{HL} = \sum_{\mathbf{l}\sigma} \sum_{\mathbf{k}\mathbf{k}'\sigma'} V_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}'-\mathbf{k})\mathbf{R}_\mathbf{l}} \hat{\nu}_{\mathbf{l}\sigma} \hat{c}_{\mathbf{k}\sigma}^{+} \hat{c}_{\mathbf{k}'\sigma'}, \qquad \hat{\nu}_{\mathbf{l}\sigma} = \hat{f}_{\mathbf{l}\sigma}^{+} \hat{f}_{\mathbf{l}\sigma}. \tag{2.4}$$

We have separated here the interaction (2.4) between the heavy and light electrons, which is fundamental in our problem, and left out the exchange part of this interaction, which does not play a decisive role in the formation of the EPE. The contribution of the allowance for the exchange interaction to the structure of the final results will be discussed separately later. As already noted, the interaction of the light electrons with one another will be neglected.

The Hamiltonian $\hat{H}'$ has the standard structure.

$$\hat{H}' = \Delta_0 \sum_{\mathbf{l}\mathbf{g}\sigma} \hat{f}_{\mathbf{l}\sigma}^{+} \hat{f}_{\mathbf{l}+\mathbf{g}\sigma}. \tag{2.5}$$

When considering hybridization, we shall understand $\hat{H}'$ in (2.1) to mean Eq. (1.9).

We begin with the case of an intersection of a narrow and a wide band. We neglect first the interband interaction U_{HH} of the electrons, and retain the interaction $\hat{H}_{HL}$ that determines the EPE. The problem is then equivalent to that

of the motion of a heavy particle in a metal (see the Introduction), and we can use the results of Ref. 1. As $\rightarrow 0$ the width of the band narrowed-down by the EPE is given by (1.4) with account taken of (1.8). The parameter γ [see (1.3)] can be obtained by directly determining the time of coherent of the spreading of a state localized at the initial instant in the unit cell $\mathbf{n} \neq 0$:

$$\psi(t=0, \mathbf{n}) = \frac{1}{N} \sum_{\mathbf{p}} e^{i\mathbf{pn}}.$$

Here

$$\psi(t, \mathbf{n}) = \frac{1}{N} \sum_{\mathbf{p}} e^{i\mathbf{pn} - i\varepsilon_{\mathbf{p}} t}$$

and the probability of observing a particle in the cell $\mathbf{n} = 0$ at the instant of time t is equal to

$$W = \frac{1}{N^2} \sum_{\mathbf{pp}'} e^{i(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'})t}.$$

For short times, expanding the exponential, we have

$$W = \frac{1}{N^2} \sum_{\mathbf{pp}'} [1 - {}^1/_2 (\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}'})^2 t^2] = 1 - \left(\frac{t}{\tau}\right)^2.$$

In the tight-binding approximation we obtain directly for lattices of cubic symmetry

$$(\tau^{-1})^2 = z(\Delta_0)_*^2, \tag{2.6}$$

where z is the number of equivalent sites in the nearest coordination spheres. Recognizing that

$$\Delta_* = 2z\zeta(\Delta_0).$$

($\zeta < 1$ is a known numerical factor for lattices of various types), we get by comparing (2.6) with (1.3)

$$\gamma \approx 1/2\sqrt{z}\zeta. \tag{2.7}$$

We point out that the reciprocal time of departure from the cell is in all cases

$$\tau^{-1} \sim \Delta_*/5.$$

As the temperature rises, the bandwidth retains the value (1.4) and (2.7) all the way to $\Omega_T \sim \gamma\Delta$. At $\Omega_T > \gamma\Delta$ the damping of the pair correlation on neighboring sites, determined by the frequency Ω_T, leads to disruption of the itinerant motion of the electrons.[1] This motion becomes now incoherent, and the probability of a transition to a neighboring cell decreases with increasing T like (apart from a coefficient of order unity)

$$W \approx 2\tilde{\Delta}_0^2(T)/\Omega_T. \tag{2.8}$$

It follows from the form of (2.8) that in the coherent-transition regime the role of the effective tunneling amplitude is played by the amplitude (1.6).

We dwell now on the case when the peak of the density of states is due to hybridization. In the case of the one-electron problem, hybridization leads to a peak having a characteristic width

$$\Gamma \approx \pi\rho_L(\varepsilon_F) v^2 \sim v^2/\varepsilon_0.$$

Let the chemical potential lie inside this peak. When the interaction $\hat{H}_{HL}$ (2.4) is turned on, the resultant EPE leads to a renormalization, described by relation (1.10), of the vertex (1.9). A direct determination (based anew on consideration of the temporal evolution of the initial localized state) of the lifetime of a particle on an atomic level at a fixed site under hybridization conditions, shows convincingly that as $T \rightarrow 0$

$$\tau^{-1} \approx \pi\rho_L(\varepsilon_F) v_*^2 \equiv \Gamma_*. \tag{2.9}$$

A self-consistent solution of (2.9) and (1.10) leads to the limiting value (1.11) of Γ_*.

At $\Omega_T > \Gamma_*$, the coherent pattern of the motion is disrupted [see (1.10)]. The electron transitions from a localized level to the continuous spectrum and back assume now the character of uncorrelated hops. The probability $W_{a\rightarrow\varepsilon}$ from an atomic level to a continuum state with energy ε actually coincides with the probability, obtained in Ref. 1, of a transition with relatively shifted levels $\xi = \varepsilon$ (if ε is measured from the energy of the atomic level). The matrix element of the transition is constructed now from the Hamiltonian (1.9) rather than (2.5), which leads simply to replacement of Δ_0 by v. The fact that the EPE is due in this case to restructuring of the wave function of the light electrons only in the initial state, as was already noted, leads simply to replacement of b by b'. As a result we have

$$W_{a\rightarrow\varepsilon} = \frac{2\tilde{v}^2(T)\Omega_T}{\varepsilon^2 + \Omega_T^2} \sqrt{\pi} \frac{|\Gamma(1 + b' + i\varepsilon/2\pi T)|^2}{\Gamma({}^1/_2 + b')\Gamma(1 + b')} e^{-\varepsilon/2T}. \tag{2.10}$$

Here

$$\tilde{v}(T) = v(\pi T/\varepsilon_0)^{b'}. \tag{2.11}$$

The total probability of departure of the electron from the level is

$$W_a = \rho_L \int d\varepsilon\, (1 - n_\varepsilon)\, W_{a\rightarrow\varepsilon}$$

$$= \frac{\sqrt{\pi}\,|\Gamma({}^1/_2 + b' + i\mu/2\pi T)|^2}{\Gamma(1 + b')\Gamma({}^1/_2 + b')} e^{-\mu/2T} \rho_L \tilde{v}^2(T). \tag{2.12}$$

It can be seen from (2.12) that the role of the level shift is now played effectively by the chemical potential μ reckoned from the position of the atomic level. At $|\mu|/T \leqslant 1$ we have $W_a \approx \pi\rho_L\tilde{v}^2$, and from a comparison with (2.9) we can conclude directly that in the case of hybridization in the presence of EPE the role of the effective matrix element is assumed by $\tilde{v}(T)$ (2.11).

If $|\mu|/T \gg 1$ (this takes place at very low or, conversely, nearly maximum occupation of the $f(d)$ levels), it follows from (2.12) that

$$W_a \approx \pi\rho_L\tilde{v}^2(T) \left|\frac{\mu}{\pi T}\right|^{2b'} \exp\left[-\frac{\mu + |\mu|}{2T}\right]. \tag{2.13}$$

The appearance of the large factor $(|\mu|/T)^{2b'}$ is due to the decrease of the polaron effect. The effective hybridization matrix element is then [cf. (2.11)]

$$\tilde{v} = v(|\mu|/\varepsilon_0)^{b'} \tag{2.14}$$

in full analogy with the results of the two-well problem.[1]

The results demonstrate the very strong influence of the inter-electron interaction via the EPE on the decrease of the energy parameters that describe the fine structure of the spectral density for hybridization.

Notwithstanding the qualitative similarity of the narrowing in the case of a narrow band and in hybridization, attention must be called to one fundamental difference. The point is that in the case of hybridization the density of states is not cut off at a definite value of the energy but, on the contrary, decreases slowly like

$$\rho(\varepsilon)\approx\Gamma_*/\pi\varepsilon^2,\quad \Gamma_*\ll\varepsilon\ll v_*. \tag{2.15}$$

This difference is manifested in the thermodynamic and kinetic properties.

The scale (1.11) of the narrowing suggests that in many cases direct overlap of the atomic states on neighboring sites (with the EPE taken into account) will yield for Δ_* (1.14) a value exceeding (1.11). In this case we return in fact to the two-band situation.

We have so far disregarded the intraband interelectron interaction, which can naturally play a significant role in the case of narrow bands. It must be pointed out, however, that the heaviest electrons produce by themselves very effective screening, and the amplitude of their scattering by one another is of atomic scale. Therefore, at least at $\nu<\nu_c<1$, the heavy-electron subsystem at $T\ll\Delta_*(\Gamma_*)$ can escape localization (Wigner crystallization, cf. Ref. 19) or magnetic ordering, and remain a Fermi liquid. We consider below only this case, assuming that the Fermi-liquid effects are less pronounced than the effects that follow from the electron-polaron narrowing of the band or of the peak of the density of states.

At high T, when effective quasilocalization of heavy electrons takes place, the interaction U_{HH} can be represented in the standard form of Hubbard repulsion at the site

$$U_{HH}=U_0\sum_{1\sigma}\hat{\nu}_{1\sigma}\hat{\nu}_{1-\sigma}. \tag{2.16}$$

3. SPECIFIC HEAT

We consider first low temperatures $T\ll\Delta$, assuming that the number of states under the Fermi level in an EPE-narrowed band of width Δ_* is comparable with the total number of ions of the transition element. By virtue of the inequality $\Delta_*\ll\varepsilon_0$ the density of states is then $\rho_H(\varepsilon_F)\gg\rho_L(\varepsilon_F)$, and the specific heat is determined in practice only by the heavy electron. In the gas approximation we have then the standard expression

$$c_v=\frac{2}{3}\pi^2\rho_H(\varepsilon_F)T\sim\frac{T}{\Delta_*}\nu\left(1-\frac{\nu}{2}\right), \tag{3.1}$$

where ν is the number of electrons per transition-element atom in the heavy-fermion band (c_v in Eq. (3.1) is also defined per atom of the transition element; this definition is adhered to hereafter).

If the density-of-states peak is the result of hybridization, the specific heat at $T\ll\Gamma_*$ is determined by a relation similar to (3.1) but with the substitution $\Delta_*\to\Gamma_*$.

With rise of temperature, relation (3.1) becomes rapidly invalid. As soon as T becomes noticeably smaller than Δ_* the electrons begin to feel the limit of the energy width of the band, and the increase of the specific heat is replaced by a decrease of c_v with increase of T. If the temperature dependence of the band width (1.1) is neglected and the width is assumed to be fixed and equal to Δ_*, we readily obtain for the specific heat at $T\gg\Delta_*$ in the gas approximation

$$c_v=\frac{z(\Delta_0)_*^2}{T^2}\nu\left(1-\frac{\nu}{2}\right)\equiv\left(\frac{\gamma\Delta_*}{T}\right)^2\nu\left(1-\frac{\nu}{2}\right). \tag{3.2}$$

It can be concluded directly from a comparison of (3.2) with (3.1) that the maximum occurs when T is close to T_*, where

$$T_*=\gamma\Delta_*.$$

The temperature dependence of $\tilde{\Delta}_0$, due to the interaction between the heavy and light interaction, can no longer be taken into account by using the relations obtained in the gas approximation. Moreover, after the onset of dynamic disruption of the band, the concept of the spectrum of coherent one-particle states becomes altogether meaningless and the heavy electron moves under conditions of strong irreversible interaction with the light electrons. All the excitations that determine in fact the specific heat now become collective and involve inevitably the light electrons.

At $T\gg T_*$, however, a thermodynamic perturbation theory can be used (see, e.g., Ref. 20), with T_*/T the small parameter. To this end we return to the Hamiltonian (2.1) and regard $\hat{H}'$ (2.5) as a perturbation. Retaining only terms quadratic in H', we have for the thermodynamic potential

$$\Omega=\Omega_0+\delta\Omega,\quad \delta\Omega=-T\int_0^\beta d\tau\int_0^\tau ds\,\langle e^{(\tau-s)\hat{H}_0}\hat{H}'e^{(s-\tau)\hat{H}_0}\hat{H}'\rangle. \tag{3.3}$$

Here Ω_0 is the thermodynamic potential of the system in the absence of a channel for tunneling of the heavy electrons, with allowance for the spin degree of freedom, while $\beta=1/T$. It is convenient to characterize the state of the Hamiltonian $\hat{H}_0$ by a set of occupation numbers $\{\nu_{1\sigma}\}\equiv\alpha$ of heavy electrons with index m that characterizes the state of the heavy electrons at fixed α. Then

$$\delta\Omega=-\int_0^{\beta/2}dx\left(\sum_{\alpha\alpha' mm'}|\langle\alpha' m'|\hat{H}'|\alpha m\rangle|^2 e^{x(E_{\alpha' m'}-E_{\alpha m})}\right). \tag{3.4}$$

The state m is determined by a set of one-electron states in the field of static defects whose role is assumed by the heavy electrons. Recognizing that the Hamiltonian $\hat{H}'$ corresponds to a transition of only one particle, *the states m and m' correspond to one and the same static configuration of heavy electrons around the tunneling particle. The presence of static defects, however, at least when scattering of light electron is taken into account in the Born approximation, does not alter the picture of the infrared divergence due to production of electron-hole pairs near a Fermi level.* This divergence is determined only by the density of the energy states near ε_F, and the electron polaron effect for a heavy-electron transition in (3.4) will hardly differ from the case of tunneling of an individual particle in a metal (see Ref. 1).

Taking the foregoing into account, we can rewrite (3.4) in the form

$$\delta\Omega=-\int_0^{\beta/2}dx\left\langle\sum_{1g\sigma}\nu_{1\sigma}(1-\nu_{1+g\sigma})\Delta_0^2\right.$$
$$\left.\times\sum_{mm'}\rho_m{}^L|\Lambda_{1+g1}^{mm'}|^2\exp\{x(E_{m'}-E_m)+x\xi_{11+g}\}\right\rangle_H, \tag{3.5}$$

where $\xi_{\mathbf{l}+\mathbf{g}} = E_{\mathbf{l}} - E_{\mathbf{l}+\mathbf{g}}$; $\hat{\Lambda}$ is the electron polaron operator whose explicit form is given in Ref. 1; ρ_m^L is the density matrix of the light electrons. The symbol $\langle \ldots \rangle_H$ denotes averaging over the configurations of the heavy electrons.

The structure of the expression contained in the angle brackets in (35) is exactly equal to the integrand of the time integral that determines the probability of the transition of a particle from cell $\mathbf{l}$ to cell $\mathbf{l}+\mathbf{g}$, if the substitution $x \to it$ is made (see Ref. 1). Therefore, using the results of Ref. 1, we obtain directly

$$\delta\Omega = -\Delta_0^2 \int_0^{\beta/2} dx \left\langle \sum_{\mathbf{l}\mathbf{g}\sigma} v_{\mathbf{l}\sigma}(1-v_{\mathbf{l}+\mathbf{g}\sigma}) \exp[-\chi(x,T) + x\xi_{\mathbf{l}+\mathbf{g}}] \right\rangle_H, \tag{3.6}$$

where the function χ is given by

$$\chi(x,T) = 2b \iint \frac{d\varepsilon\, d\varepsilon'}{(\varepsilon-\varepsilon')^2} n_\varepsilon (1-n_{\varepsilon'})(1-e^{x(\varepsilon-\varepsilon')}). \tag{3.7}$$

In this expression b is defined according to (1.2), and n_ε is the Fermi distribution of the electrons. Since $T \ll \varepsilon_F$, expression (3.7) can be transformed into

$$\chi(x,T) = 2b \int_0^{\varepsilon_0} \frac{dy}{y} \frac{\operatorname{ch} y/2T - \operatorname{ch}(yx - y/2T)}{\operatorname{sh} y/2T}. \tag{3.8}$$

Expression (3.6) was written for a metal with arbitrary distribution of the static level deviations between the cells and makes it possible, in principle, to take into account both the influence of the deviation of the crystal from ideal and the electron-electron interaction in the narrow band (in the latter case it is necessary to take into account the dependence of $\xi_{\mathbf{l}+\mathbf{g}}$ on the distribution of the occupation numbers α). If the relative level deviations on going over to the free cell are $\xi_{\mathbf{l}+\mathbf{g}} \ll T$, and on the contrary, for a transition to a cell occupied by an electron with an arbitrary spin projection we have according to (2.16) $\xi_{\mathbf{l}+\mathbf{g}} \approx U_0 \gg T$, the averaging in (3.6) becomes trivial. As a result we get for the correction to the thermodynamic potential per transition-element atom

$$\delta\Omega = -z\Delta_0^2 v(1-v) \int_0^{\beta/2} dx\, e^{-\chi(x,T)}. \tag{3.9}$$

Calculating this integral, we obtain ultimately ($\varepsilon_0 \gg T$)

$$\delta\Omega = -\frac{z\bar{\Delta}_0^2(T)}{T} v(1-v) \frac{\Gamma(1/2-b)}{2\sqrt{\pi}} \left(1 - \left(\frac{T}{\varepsilon_0}\right)^{1-2b}\right) \tag{3.10}$$

(the last factor is retained only to be able to take correctly the limit as $b \to 1/2$).

We have accordingly for the specific heat

$$c_v = \frac{z\bar{\Delta}_0^2(T)}{T^2}(1-b) \frac{\Gamma(3/2-b)}{\Gamma(3/2)} v(1-v) \sim \left(\frac{T_*}{T}\right)^{2(1-b)} v(1-v). \tag{3.11}$$

Note that in the considered high-temperature limit the thermodynamic potential Ω_0 in (3.3) corresponds to a large spin entropy $s_0 = \ln 2$, but the corresponding specific heat is equal to zero. As a result, the total specific heat appears only as a result of tunnel motion and is determined by (3.11). At $\varepsilon_0 \gg \Delta_*$ the value v varies very little with T, and we shall neglect this variation. As $b \to 0$, Eq. (3.11) takes the form (3.2) except that for a noninteracting fermion gas we have in (3.2) the factor $(1 - v/2)$ in place of the $(1 - v)$, in (3.11) when account is taken of the Hubbard interaction (2.16). If we put $U_0 = 0$ initially in the calculation of (3.6), the factor $(1 - v/2)$ is restored.

The presence of the EPE leads to a decrease of the specific heat with increase of T, given by

$$c_v \sim 1/T^{2(1-b)}.$$

The exponent depends now on the electron-electron interaction and ranges from 1 to 2. The slower decrease of c_v compared with (3.2) is due to the decrease of the polaron effect with increase of T and by the same token to the increase of the effective amplitude of the tunneling transition (1.6).

Comparison of (3.11) with (3.1) show that the specific heat reaches, as before, a maximum at a low temperature of the order of $T_* < \Delta_*$.

We consider now the high-temperature behavior of the specific heat in the case of hybridization. If $\Omega_T \gg \Gamma_*$ the interaction between the heavy and light electron again makes the concept of one-particle states of heavy electrons at the density peak meaningless. To find the specific heat in this case we use the thermodynamic perturbation theory in the form (3.3), taking $\hat{H}'$ to be the Hamiltonian (19) and using the small parameter Γ_*/T. Now α' in (3.4) differs by one absorbed (created) f (d) electron, and m' differs from m by one created (absorbed) light electron $\mathbf{k}$ and by a definite number of electron-hole pairs that appear when the polaron jacket is shaken-up. All the arguments used for the transition from (3.4) to (3.5) remain in force, and a change of the state of one light electron influences little polaron effect (see the remark pertaining to Eq. (1.11)). Assuming that the inhomogeneous spread of the levels is small compared with T, and that $U_0 \gg T$, we have in place of (3.6)

$$\delta\Omega = -2\rho_L v^2 \int_0^{\beta/2} dx \int_{-\varepsilon_0}^{\varepsilon_0} d\varepsilon \left[\frac{v}{2}(1-n_\varepsilon)e^{-x\varepsilon} + (1-v)n_\varepsilon e^{x\varepsilon}\right] e^{-\chi(x,T)}. \tag{3.12}$$

The form of the expression in the square brackets corresponds to a strong Hubbard repulsion on the localized atomic level, and accordingly

$$v = (1 + 1/2 e^{-\mu/T})^{-1}. \tag{3.13}$$

In (3.12), ε is reckoned from the energy ε_a of the atomic level, and $\mu = \varepsilon_F - \varepsilon_a$. The symmetric limits in the integral over $d\varepsilon$ were chosen only for simplicity. The expression for $\chi(x,T)$ in (3.12) differs from (3.8) in that b is replaced by b'.

By making the integrals dimensionless, we get after simple transformations

$$\delta\Omega = -\rho_L v^2 v \int_0^{1/2} d\xi\, e^{-\chi(\xi,T)} J\left(\xi, \frac{\varepsilon_0}{T}\right), \tag{3.14}$$

$$J\left(\xi, \frac{\varepsilon_0}{T}\right) = \int_{-\varepsilon_0/T}^{+\varepsilon_0/T} dz \frac{e^{z(1-\xi)} + e^{z\xi}}{e^z + e^{\mu/T}} \qquad (\xi = xT). \tag{3.15}$$

Assuming that $\varepsilon_0 \gg \Gamma_*$, we can neglect the change of the population of the atomic levels with change of temperature. In

other words, we can assume that ν and the ratio μ/T remain unchanged. Taking this into account, we determine the entropy correction $\delta S = -\partial\delta\Omega/\partial T$.

We use the fact that with exponential accuracy with respect to the parameter $\varepsilon_0/T \gg 1$ we have

$$-\frac{\partial}{\partial T}\chi(\xi, T) \approx \frac{2b}{T}(1-e^{-\xi\varepsilon_0/T}) \equiv B(\xi, T),$$

$$\frac{\partial}{\partial T} J\left(\xi, \frac{\varepsilon_0}{T}\right) \approx -\frac{\varepsilon_0}{T}(1+e^{-\mu/T})e^{-\xi\varepsilon_0/T} \equiv -\frac{1+e^{-\mu/T}}{2b}\frac{\partial B}{\partial \xi}.$$

Differentiating (3.14) with respect to T and transforming the resultant integral with allowance for these relations and (3.13), we get

$$\delta S \approx -2\rho_L v^2\left(1-\frac{\nu}{2}\right)\left\{\frac{e^{-\chi(1/2,T)}}{T} + \int_0^{1/2} d\xi\, e^{-\chi(\xi,T)} \times\left[\frac{\partial\chi(\xi,T)}{\partial\xi}\frac{B}{2b} - BJ\left(\xi, \frac{\varepsilon_0}{T}\right)\right]\right\}. \tag{3.16}$$

Here

$$\chi(1/2, T) \approx 2b' \ln(\varepsilon_0/\pi T). \tag{3.17}$$

The first term in (3.16) determines the high-temperature correction to the entropy on account of hybridization, into which the electron-electron interaction enters by virtue of the polaron-induced decrease of the hybridization amplitude $\tilde{v} = v\exp\{-1/2\,\chi(1/2,T)\}$ ⟨see (2.11)⟩. As $b\to 0$ this correction remains finite. The second term in (3.16) is due entirely to the interaction between the heavy and light electrons, and it vanishes as $b'\to 0$. The integral over $d\xi$ in (3.16) is well defined as $\xi\to 0$ and (3.5) we can, in the range between the integration limits of (3.15) and (3.16), substitute $\varepsilon_0/T\to\infty$ in the expression in the square brackets of the integrand. On the other hand, to the same degree of accuracy,

$$\chi(\xi, T) = \chi(1/2, T) + 2b'\int_0^\infty \frac{dy}{y}\frac{1-\mathrm{ch}\,(1-2\xi)y}{\mathrm{sh}\,y}$$

$$= \chi(1/2, T) + 2b' \ln\sin\pi\xi.$$

As a result we obtain ultimately by direct calculation

$$\delta S \approx -2\rho_L\tilde{v}^2(T)(1-\nu/2)T^{-1}(1+A(\nu, b')),$$

$$A(\nu, b') = 2\pi b'\int_0^{1/2}\frac{d\xi}{(\sin\pi\xi)^{1+2b'}}\left[\cos\pi\xi - \frac{\mathrm{ch}\,(\mu(1-2\xi)/2T)}{\mathrm{ch}\,(\mu/2T)}\right]. \tag{3.18}$$

The value of μ/T is easily expressed from (3.13) in terms of ν. Note that (3.18) can be easily generalized to include arbitrary values of U_0. In particular, at $U_0 = 0$ it suffices to make in (3.18) the substitutions

$$1-\frac{\nu}{2}\to 1, \qquad \frac{\mu}{T}\to \ln\left(\frac{\nu}{2-\nu}\right). \tag{3.19}$$

It is easily verified that at $b' \leqslant 1/4$

$$A(\nu, b') > -1$$

and the sign of δS is uniquely determined.

Just as in the case of a narrow band, the specific heat is connected only with the obtained correction to the entropy, and vanishes identically in the absence of hybridization.

From (3.18) we get

$$c_v \approx \frac{2\rho_L\tilde{v}^2}{T}\left(1-\frac{\nu}{2}\right)(1-2b')(1+A(\nu, b')). \tag{3.20}$$

The specific heat now decreases with temperature like

$$c_v \sim (\Gamma_*/T)^{1-2b'}, \tag{3.21}$$

i.e., much more slowly than in the case of a narrow band. For $b' = 0$ we have

$$c_v = \frac{2\rho_L v^2}{T}\left(1-\frac{\nu}{2}\right) \sim \frac{1}{T}.$$

It can be seen that the electron-electron interaction can alter noticeably the character of the decrease of c_v with T, especially when the parameter b' is close to the limiting value 1/4.

It is of formal interest to analyze the specific heat in the case of hybridization when ν is close to 0 or 1. As $T\to 0$ the chemical potential μ_0 is in this case outside the energy interval $\sim\Gamma_0$. At high temperature, which is now defined by the condition $T \gg |\mu_0|, \Gamma_*$, the connection between ν and μ will be determined as before by relation (3.13), from which follows the inequality $T \gg 1$. In this case the region of small $\xi \sim T/|\mu|$ becomes significant in the integral (3.18) that defines $A(\nu, b')$. Direct calculation yields

$$A(\nu, b') \approx \frac{2\pi b'|\mu/T|^{2b'}}{\sin(2\pi b')\Gamma(1+2b')}.$$

Assuming here that $A \gg 1$, we see that the value of the effective hybridization is changed from (2.11) into (2.14). This is natural since, as we have already noted, μ plays the role of the relative collapse of the levels in the two-well problem. Note that by virtue of the linear relation $\mu \sim T$ the form of the temperature dependence (3.21) remains the same.

Thus, the electron-electron interaction due to the EPE leads to the following general picture of the temperature dependence of the specific heat in the case of a narrow band or a narrow peak of the density of states in the case of hybridization. At low temperatures, the anomalously rapid linear increase of c_0 with T, due to the large effective mass m, gives way to a decrease already at $T \sim T_*, \Gamma_*$ [see Eqs. (1.4) and (1.11)]. In this case c_v decreases as the power law $c_v \sim T^{-n}$, where the exponent depends on the interaction between the heavy and light electrons and has a value between 1 and 2 in the case of a narrow band [see (3.11)] and between 1/2 and 1 in the case of hybridization. The decrease will continue until the phonon specific heat, which increases with temperature, becomes larger than the electronic specific heat. The $c_v(T)$ dependence takes qualitatively the form shown in Fig. 1. The peak of the temperature dependence of the specific heat will become more strongly pronounced the smaller T_* or Γ_* compared with the Debye temperature Θ_D. At comparable values of these parameters, only a nonmonotonic growth of $c_v(T)$ can remain.

The results in this section were obtained neglecting the exchange interaction between the heavy and light electrons, and by the same token the possible manifestation of the Kondo effect. If the exchange interaction is turned on, its

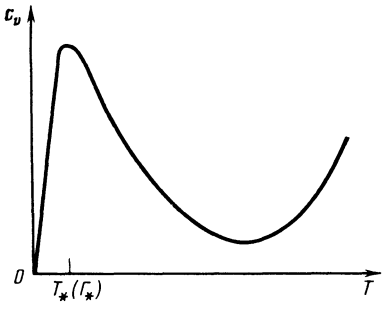

FIG. 1.

role at low temperatures will depend on the relation between Δ_*, Γ_*, and the Kondo temperature T_K that would obtain at $\Delta_*, \Gamma_* = 0$. We assume here that the itinerant motion of the heavy electrons prevents the appearance or a substantial manifestation of the Kondo effect.

At high T the increase of the probability of electron departure from the atomic level (2.12) with increase of T will continue to hinder, in the case of hybridization, the determination of the local spin properties of heavy electrons. In the case of the narrow band at $\Omega_T \gg \gamma\Delta_*$, however, the slowing down of the diffuse motion of the heavy electron [see (2.8)] causes the light electrons to begin to be scattered by the heavy ones practically in the same manner as by immobile spin-possessing impurities. This should lead in principle to an independent addition Δc_s to the specific heat; in contrast to (3.11), this addition does not vanish if $\Delta_0 = 0$ is assumed. The independence of these spins at high temperatures yields a value of Δc_s that is apparently close to that obtained for an individual impurity at $T \gg T_K$ (see, e.g., Ref. 21), multiplied by ν. This addition decreases with increase of T and the general form shown in Fig. 1 for the $c_v(T)$ dependence remains in force.

A few words concerning the role of defects. If their density is appreciable, static disruption of the band sets in, and as $T \to 0$ the heavy electrons become localized. This takes place at a characteristic atomic-level spread $\varepsilon_0 \gg \delta E > \Delta_*(\Gamma_*)$. The specific heat at low temperatures $T \ll \delta E$ retains the form (3.1), with Δ_* and Γ_* replaced by δE. At high $T \gg \delta E$ the specific heat differs from zero even in the zeroth approximation in Δ_0 and v. In this case $c_v^{(0)}$ decreases as before with T in power-law fashion:

$$c_v^{(0)} \sim (\delta E/T)^n, \tag{3.22}$$

where $n = 2$ or 1 for a Gaussian and Lorentzian level distribution, respectively. It is easy to conclude from a comparison of this result with (3.11) and (3.20) that in the case $n = 2$ the specific heat begins to be governed by the hopping of the heavy electrons at $\tilde{\Delta}(T) > \delta E$ in the itinerant regime and at $T\,\tilde{\Gamma}(T) > \delta E$ under hybridization conditions. At $n = 1$ the static spread always plays the predominant role in the itinerant case, and in the case of hybridization the transition to (3.20) takes place at $\tilde{\Gamma}(T) > \delta E$.

4. MAGNETIC SUSCEPTIBILITY. DEPENDENCE OF c_v ON THE MAGNETIC FIELD

Consider the susceptibility at low temperature, taking account in the electron-electron interaction only the leading term of $\hat{H}_{HL}$ (2.4). For the EPE-narrowed band we have then at $T \ll T_*$ an expression typical of the gas approximation:

$$\chi = 2\mu_m^2 \left[\rho_H(\varepsilon_F) + \frac{\pi^2}{6} T^2 \left(\rho_H''(\varepsilon_F) - \frac{\rho_H'^2(\varepsilon_F)}{\rho_H(\varepsilon_F)} \right) \right], \tag{4.1}$$

where μ_m is the magnetic moment of the f (d) electron. As a rule $\rho_H''(\varepsilon_F) < 0$, so that the susceptibility as a whole decreases with increase of T, although the true behavior depends in principle on the position of ε_F relative to the bottom of the band.

With further increase of T, the principal role is assumed by the finite character of the width Δ_* of the band and its dynamic disruption. The site representation becomes adequate, and the heavy electrons become quasilocalized. The magnetic susceptibility differs now from zero even in the zeroth approximation in Δ_0, when it reduces simply to the Curie law

$$\chi_0(T) = \frac{\mu_m^2}{T} \begin{cases} \nu(1-\nu/2) & U_0 = 0 \\ \nu & U_0 = \infty \end{cases}. \tag{4.2}$$

The hopping correction to the susceptibility can be obtained from expression (3.6) in which, however it is necessary to determine the dependence of the quantity

$$1/N \left\langle \sum_{\mathbf{l}g\sigma} \nu_{l\sigma}(1-\nu_{l+g\sigma}) \exp(\xi_{l+g}/T) \right\rangle$$

on the magnetic field. It is readily found that this mean value is equal to

$$z\nu(1-\nu/2) - {}^1\!/_2 z(\mu_m H/T)^2 (\nu(1-\nu/2))^2, \quad U_0 = 0.$$
$$z\nu(1-\nu) \qquad U_0 = \infty$$

It follows therefore that the correction Δ_χ to (4.2) is altogether nonexistent in this approximation in the case of strong Hubbard repulsion, while at $U_0 = 0$ it is equal to

$$\Delta\chi = -\frac{\mu_m^2}{T} \frac{z\tilde{\Delta}_0^2(T)}{T^2} (\nu(1-\nu/2))^2 \times \frac{\Gamma({}^1\!/_2 - b)}{2\sqrt{\pi}} (1-(T/\varepsilon_0)^{1-2b}). \tag{4.3}$$

The change to the Curie law (4.2) takes place at higher temperatures than the change to that branch of the c_v dependence which decreases with temperature, although as $T \to 0$ the ratio $c_v(0)/T_\chi(0)$ is close to the gas ratio. It must be stated that this circumstance is typical of the behavior of heavy-fermion systems (see, e.g., Refs. 12 and 13). Note that in real systems the Curie law changes into the Curie-Weiss law, for a large number of reasons. In particular, this may be due to the crystal splitting of the degenerate narrow band,[12] to indirect interaction between quasi-localized spins via the light electrons, and others.

The results presented remain in force, naturally, also in the case of hybridization. All that changes is the expression for Δ_χ, which takes now the form

$$\Delta\chi = -\frac{\mu_m^2}{T} \frac{\pi\rho_L\tilde{v}^2}{T} \nu \int_0^{1/b} \frac{d\xi\, \xi(1-\xi)}{(\sin(\pi\xi))^{1+2b'}} [e^{(\xi-1)\mu/T} + e^{-\xi\mu/T}]. \tag{4.4}$$

This general relation is valid both for $U_0 = 0$ and for $U_0 = \infty$, depending on whether the relation between μ and ν is given by (3.13) or (3.19).

A quantity frequently measured is dc_v/dH. It is easy to show that the following thermodynamic relation holds:

$$dc_v/dH = Td^2M/dT^2.$$

Using expressions (4.1) and (4.2), we verify that at high T we always have $dc_v/dH > 0$, and at low ones, conversely, almost always $dc/dH < 0$. This behavior is also typical of heavy-fermion systems.[12,13] Note that since this result is not connected with the electron polaron effect, it was understood even earlier that the reversal of the sign of dc_v/dH can be explained by assuming the presence of a very narrow band (see Ref. 12 and the citations therein).

5. RESISTIVITY

In contrast to the thermodynamic characteristics, a contribution to the conductivity of the systems considered is made by both heavy and light electrons. The conductivity of the light electrons is decisively governed by their scattering from heavy electrons. Direct calculation of $\sigma(T)$ at $T \ll \Delta$ yields, within the framework of the quasiclassical transport equation,

$$\sigma(T) = \sigma_0 \Delta_*^2/T^2. \tag{5.1}$$

Here σ_0 is close to the conductivity of the light-electron band, when the heavy electrons assume the role of randomly distributed static defects.

The conductivity of the heavy-electron band, with allowance for their scattering by one another and by the light electrons, is given by an expression similar to (5.1). The reason is that the amplitude of the scattering of light electrons by heavy ones and of heavy ones by one another have an interatomic-distance scale a of the same order, and the ratio τ_H/m_H (τ_H is the heavy-electron relaxation time) is practically independent of the effective mass.

At $T \gg T_*$ the light electrons are actually scattered by the heavy ones as by static defects. Their conductivity approaches then a constant value $\sigma_{L\infty}$, which close in order of magnitude to ∞.

In the dynamic band disruption regime $\Omega_T > T_*$ the heavy electrons continue to move diffusely. The decisive factor in this case is their interaction with light electrons, which was indeed the cause of the band disruption and of the appearance of transport formally with a mean free path $l < a$ (cf. Refs. 8 and 9). The hopping probability and the associated diffusion coefficient D (Ref. 1) decrease in this case slowly with temperature.

Using the known connection between the conductivity and D, and taking into account the strong Hubbard repulsion at the site, we get

$$\sigma_H = e^2 n_0 \nu(1-\nu)\frac{a^2}{3}\frac{z\tilde{\Delta}_0^2(T)}{T\Omega_T} = \sigma_H^0\left(\frac{\Delta_*}{T}\right)^{2-2b}, \tag{5.2}$$

where n_0 is the density of the transition-element atoms. The expression for σ_H^0 is similar to that for $\sigma_{L\infty}$ or σ_0 but its numerical value can be noticeably smaller.

Note that $\sigma_{L\infty}$ is given by the same relation

$$\sigma_{L\infty} \sim \nu(1-\nu),$$

in view of the fact that the light electrons are scattered only to the extent that the heavy electrons are randomly distributed. It is easily understood that if ν lies somewhat between 0 and 1, $\sigma_{L\infty}$ is close to the limit corresponding to the so-called "minimum metallic conductivity." The resistivity ρ will thus increase quadratically with T very rapidly at low temperatures, in an interval $\sim T_*$, reaching a value close to $\rho_{\max}$. At high temperatures ρ will continue to grow slowly, now in accordance with

$$\rho = \rho_{L\infty}(1-\alpha(\Delta_*/T)^{2-2b}), \quad \alpha = \sigma_H^0/\sigma_{L\infty}. \tag{5.3}$$

The behavior pattern is shown qualitatively in Fig. 2 (curve a).

In the case of the model with hybridization, the temperature dependence of the conductivity at $T \ll \Gamma_*$ retains the form, with the natural replacement $\Delta_* \to \Gamma_*$. The value of σ again decreases to close to $\sigma_{\min}$ in a narrow temperature interval on the order of Γ_*. At high temperatures $T \gg \Gamma_*$, however, the character of the $\sigma(T)$ dependence for hybridization will differ substantially from the case of a narrow band. The reason is that at $\Omega_T \gg \Gamma_*$ we have not only disruption of the itinerant motion at the density peak and quasilocalization of the heavy electrons but an opening of an addition incoherent scattering channel for the light electrons, due to their capture by free atomic levels. Let us examine this question in more detail.

The probability of a transition of an electron from an atomic level to the state of a continuous spectrum with energy ε is determined by Eq. (2.10). This enables us to write down right away an expression for electron capture from the continuum, using the detail balancing principle. The reciprocal relaxation time $\tau_c^{-1}(\varepsilon)$ for this inelastic scattering channel, which enters in the transport equation for light electrons, can be written in this case in the form

$$\tau_c^{-1}(\varepsilon) = W_{a\to\varepsilon}(\nu/2)\,(1+e^{(\varepsilon-\mu)/T}). \tag{5.4}$$

We denote by τ_∞ the relaxation time corresponding to scattering of a Langmuir electron by randomly located defects, whose role is assumed by localized heavy electrons. It is easy to estimate that

$$\tau_\infty/\tau_c \sim \rho_L \tilde{v}^2(T)/\Omega_T \ll 1.$$

From this we have for the total relaxation time τ the value

$$\tau = \tau_\infty(1-\tau_\infty/\tau_c),$$

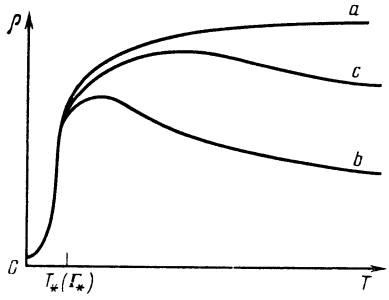

FIG. 2.

and the high-temperature expression for the resistance takes the form

$$\rho=\rho_{L\infty}\left(1+\xi'(\nu,b')\frac{\rho_L\tilde{v}^2(T)}{T}\right)$$
$$=\rho_{L\infty}\left(1+\xi(\nu,b')\left(\frac{\Gamma_*}{T}\right)^{1-2b'}\right), \qquad (5.5)$$

where ξ' and ξ are coefficients independent of T.

We see that, in contrast to the narrow band, the resistivity at high temperatures decreases with increase of T. The resistivity goes thus through a maximum with a value on the order of the maximum metallic resistivity $\rho_{\max}$, and then falls off rapidly with increase of T, in contrast to the very rapid increase at low T. The transition region experience a lag on the low temperature side as $\tilde{\Gamma}(T)$ increases with T, and the general form of $\rho(T)$ is shown by curve b of Fig. 2.

In the analysis of the two-band model we have implicitly assumed that the inequality $\Gamma_* \sim v_*^2/\varepsilon_0 \ll \Delta_*$ is valid and have neglected the hybridization completely. The difference in the character of the temperature dependences of the resistivity (5.3) and (5.5) predetermines, however, even in this case the possibility that $\delta\rho(T)$ can go over at high T from the two-band to the hybridization regime. If it is recognized that at $\Omega_T \gg \Delta_*, \Gamma_*$ the channel of heavy-electron motion through a straight band and the hybridization channel causing capture of the light electron by a level are independent, it is possible to write in this high-temperature level a general expression for the resistivity, in the form

$$\rho=\rho_{L\infty}(1-\alpha(\Delta_*/T)^{2-2b}+\xi(\Gamma_*/T)^{1-2b'}). \qquad (5.6)$$

The result may be the $\rho(T)$ dependence shown in Fig. 2 (curve c), a feature of which is the appearance of a highly stretched-out gently sloping maximum (plateau).

Note that a similar change of the regime, with transition from (3.11) to (3.20) under certain condition, takes place in fact also for the specific heat.

Allowance for the exchange interaction at high temperatures includes an additional spin channel for scattering of light electrons by quasilocalized heavy electrons. This channel should lead to a resistivity increment $\delta\rho_s$ with the logarithmic temperature dependence typical of the Kondo effect, whose sign is determined by the sign of the exchange interaction. Note that the weak logarithmic dependence of $\delta\rho_s(T)$ at a bounded value of the exchange interaction leaves qualitatively unchanged the form of the resistivity temperature dependence shown in Fig. 2.

Note that the presence of zero-spin defects has little effect on the high-temperature branch of the resistivity (5.3), (5.5), since the temperature disruption of the heavy-electron band leads already to their quasilocalization.

Typical of many measurements of $\rho(T)$ in metallic systems with heavy electrons (see, e.g., the literature cited in Refs. 11–15) is the behavior of the curves of Fig. 2. Thus, in the case of A-15 compounds the picture observed is qualitatively close to curve a of this figure (see Refs. 14 and 15). Metallic compounds of rare-earth elements and actinides are more likely to have $\rho(T)$ decrease with increase of T at high temperatures (curves b and c), and the maximum of the resistivity has most frequently the form of a quasi-plateau.

According to (3.11) and (5.3), and also (3.20) and (5.5), the temperature dependences of the specific heat and the corrections to the resistivity coincide in the region of high T. This circumstance can be directly verified in experiment.

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