

# Spin fluctuations and heavy fermions in the Kondo lattice

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This paper studies the spectrum of the spin and electronic excitations of the Kondo lattice at low temperatures. To avoid unphysical states, the Mattis “drone”-fermion representation for localized spins is employed. First, the known Fermi liquid properties of a single impurity are examined. The behavior of the correlator between a localized spin and the electron spin density at large distances shows that the effective interaction between electrons on the Fermi level and low-energy localized spin fluctuations scales as  $\rho^{-1}$ , where  $\rho$  is the band-state density. This fact is developed into a renormalization of the band spectrum in a periodic lattice. If the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction between localized spins is much smaller than the Kondo fluctuation frequency  $\omega_k$ , the temperature of the crossover to the single-parameter Fermi liquid mode is determined by  $\omega_k$ . When the RKKY interaction becomes of order  $\omega_k$ , there is a new scale  $\omega_{sf}$ , the energy of the (antiferromagnetic) paramagnon mode, with  $\omega_{sf} \ll \omega_k$ . Here the coherent Fermi liquid regime is realized only below a temperature  $T_{\text{coh}}$  of order  $\omega_{sf}$ , while above  $T_{\text{coh}}$  quasiparticle damping exhibits a linear temperature dependence. Finally, the nuclear-spin relaxation rate is calculated.

## 1. INTRODUCTION

The idea of a heavy-fermion state as a Fermi liquid “fixed point” of the Hamiltonian of the Kondo lattice model is widespread. But the procedure by which the low-energy limit is attained in this model is yet to be clarified in the technical aspects (a general review of this topic can be found, e.g., in Refs. 1 and 2). In the popular  $1/N$ -theory ( $N$  is the degree of degeneracy of a localized state) introduced into this problem in Refs. 3–6, the “heavy” band emerges even in the mean-field approximation ( $N = \infty$ ) as the result of coherent hybridization of the broad conduction band and localized pseudofermions, introduced to describe the spin degrees of freedom of the  $f$  shell of rare-earth ions. It is assumed that this result can be qualitatively interpolated to the physical limit with  $N=2$ , which corresponds to the canonical Kondo model with spin  $\frac{1}{2}$ , although certain aspects appear unclear from the physical viewpoint. For instance, the  $1/N$ -theory predicts a dramatic alteration in the topology of the Fermi surface (this result was recently debated in Ref. 7) and leads to an insulator state of the Kondo lattice of any dimensionality in the case of a half-filled conduction band. The latter is understandable for  $\lambda = J\rho > 1$  (here  $J$  is the sf exchange coupling constant, and  $\rho$  the band-state density at the Fermi level), whereupon the problem reduces<sup>8</sup> to the Hubbard model with localized Zhang–Rice singlets.<sup>9</sup> However, for  $\lambda \ll 1$  such a critical dependence of the nature of the ground state of the nonmagnetic Kondo lattice on the total number of electrons in the band appears remarkable, except in low-dimensional systems. Undoubtedly, the insulator gap appears in a half-filled one-dimensional Kondo lattice<sup>10–12</sup> for an arbitrary coupling constant  $\lambda$ , but this result is a natural consequence of the fact that the problem is one-dimensional. Possibly, the insulating hybridization (pseudo)gap in a three-dimensional Kondo lattice is an artefact of the  $1/N$ -theory, in which the passage to the physical limit of  $N=2$  brings to

light the involved problem of excluding the superfluous states that appear while working with spin operators. The effectiveness of the  $1/N$ -theory in the impurity problem is unquestionable (see the review paper of Bickers<sup>13</sup>); it appears, however, that a satisfactory solution to the delicate problem of mutual adiabatic correspondence between the spectra for the limit values  $N = \infty$  and  $N=2$  in the three-dimensional Kondo lattice has yet to be found.

An attempt to bypass the problem of unphysical states in “hybridization” theories was recently made by Tsvetlik<sup>14</sup> and Coleman *et al.*<sup>15</sup> who used the representation of spin atoms in terms of real (Majorana) fermions.<sup>16</sup> By also expanding the band-state creation operators in terms of Majorana components Coleman *et al.*<sup>15</sup> found a mean-field solution corresponding to a superconducting state. Here the scale of the order parameter is determined by the Kondo temperature, a natural consequence of the factorization of the Kondo interaction. However, the ansatz of Ref. 15 leads to an undesirable asymmetry of the band spectrum in spin and, more important, leaves the question of the properties of the normal “heavy-fermion” phase unresolved.

Another approach to the heavy-fermion problem, apparently originating in the papers of Razafimandimby *et al.*<sup>18</sup> and Varma<sup>18</sup> (see also Eliashberg’s paper<sup>19</sup>), are based on the localized Fermi liquid picture of Nozieres<sup>20</sup> for a single Kondo impurity. The picture assumes that for  $T \ll T_k$  the internal spin degrees of freedom are frozen; elastic scattering on a Kondo center, which in the single-impurity approximation leads to the unitary limit in resistivity, plays no role in a regular lattice because of the Bloch theorem. Also, a local and highly retarded interaction arises between electrons due to the exchange of virtual spin excitations of the Kondo complex, an exchange that ensures the dynamic increase in the mass of the carriers. The spin excitations themselves contribute to the entropy in a Fermi liquid form, further increasing the effective “thermodynamic” mass (see also the discussion

in Ref. 7). To this second approach we can also refer the variants of single-site approximations in the Kondo lattice, in which the self-energy of localized  $f$ -states is assumed the same as for a single impurity<sup>21</sup> and the RKKY interaction between spins is taken into account separately, in various approximations.<sup>22,23</sup>

This paper studies the low-temperature behavior of a Kondo lattice without resorting to homogeneous hybridization of states and following the ideology of the second approach. We will find the spectrum of localized spin fluctuations and the scattering amplitude for conduction electrons by analyzing the single-impurity case. Then we will renormalize the electron spectrum in the lattice, following the work of Varma<sup>18</sup> and Éliashberg.<sup>19</sup> As a result we will find that the spectra of both spin and charge excitations are characterized by a single parameter  $\omega_k$ . Such universal behavior is actually exceptional from the experimental point of view. Even the normal (nonmagnetic and nonsuperconducting) phase of a Kondo system exhibits crossover behavior at what has become known as the coherence temperature  $T_{\text{coh}} < \omega_k$ . Only below this temperature does a true Fermi liquid picture emerge<sup>24–26</sup> (the quadratic resistivity law, the Korringa law of nuclear spin relaxation, positive magnetoresistance, etc.). Here the ratio  $T_{\text{coh}}/\omega_k$  strongly varies with substance within a broad interval. Experiments in neutron scattering show<sup>27</sup> that interstitial spin correlations, strengthening as the temperature lowers, reach saturation as temperatures of the order of  $T_{\text{coh}}$  are approached. The emergence of this new characteristic temperature (in addition to  $T_k$ ) distinctly sets the Kondo lattice apart from the impurity case, where the temperature at which the Fermi liquid mode is entered is controlled, as is known, by the Kondo fluctuation frequency  $\omega_k$ . Although the RKKY interaction obviously also participates in the coherence mode as it becomes established in the lattice, a generally accepted theory relating the temperature  $T_{\text{coh}}$  to the scale of the RKKY interaction and the frequency  $\omega_k$  has yet to be developed. This paper shows that the spin-spin RKKY interaction leads to the appearance of a collective relaxation mode of a ferromagnetic or antiferromagnetic nature, provided that the interaction is close in strength to  $\omega_k$  (the system is close to a magnetic transition). The spectral weight of these excitations is concentrated at low frequencies,  $\omega_{sf} \sim \omega_k - \omega_{\text{RKKY}}$ . If, by way of an example, we calculate the paramagnon-related contribution to the decay of electronic states and the Korringa relaxation rate, we establish that Landau's Fermi liquid picture is achieved only at low temperatures  $T \sim \omega_{sf}$ , when the (anti) ferromagnetic correlations between spins cease to be temperature-dependent.

The plan of the paper is as follows. Section 2 is devoted to spin correlators for a single Kondo impurity. In Sec. 3 we will investigate the formation of the "heavy" band of current carriers in the lattice. Section 4 takes into account the effects of the RKKY interaction on the establishment of the coherent mode. Finally, Sec. 4 is devoted to a discussion of the results.

## 2. A SINGLE KONDO IMPURITY

The Hamiltonian of the Kondo problem is

$$H = \sum_{k\sigma} \xi_k c_{k\sigma}^+ c_{k\sigma} J(S_i \sigma_i), \quad (1)$$

where  $c_{k\sigma}^+$  is the creation operator of a band state with energy  $\xi_k$ , and  $\sigma_i$  the operator of the conduction-electron spin density at a site  $i$  where the localized spin  $S = \frac{1}{2}$  is found. To avoid the Gutzwiller projection procedure, unavoidable in the usual pseudofermion representation of a spin operator, we use an approach close to the one employed in Refs. 14 and 15. More exactly, we write the impurity spins in the form suggested by Mattis:<sup>28</sup>

$$S^z = f^+ f - \frac{1}{2}, \quad S^+ = f^+ \chi, \quad S^- = \chi f, \quad (2)$$

where  $f$  and  $f^+$  are Fermi operators, and the real (Majorana) operator  $\chi = \chi^+$ , defined by the relation  $\{\chi_i, \chi_j\} = \delta_{ij}$ , ensures the correct commutation of spins at different sites and with the conduction-electron operators. According to Eq. (2), the state of a spin with a projection  $\frac{1}{2}(-\frac{1}{2})$  corresponds to the presence (absence) of an  $f$ -fermion. Representation (2) transforms into the one used by Coleman *et al.*<sup>15</sup> if  $f$  and  $f^+$  are replaced by two Majorana fermions.

To within unessential constants, the exchange interaction of localized spins with conduction electrons in (1) can be represented as

$$H = -J(a_i^+ a_i + b_i^+ b_i), \quad (3)$$

$$a_i = \left( f_i^+ c_{i\uparrow} + \frac{\chi_i c_{i\downarrow}}{\sqrt{2}} \right) \frac{1}{\sqrt{2}}, \quad b_i = \left( f_i^+ c_{i\downarrow} - \frac{\chi_i c_{i\uparrow}}{\sqrt{2}} \right) \frac{1}{\sqrt{2}}.$$

Here  $c_{i\sigma}$  is the annihilation operator of the current carrier in the tight binding representation:

$$c_{i\sigma} = \sum_k c_{k\sigma} \exp(ikR_i). \quad (4)$$

After (3) is factored by means of the Hubbard–Stratonovich transformation, the partition function is reduced to a functional integral over the Fermi fields  $f$ ,  $\chi$ , and  $c_\sigma$  and the auxiliary Bose fields  $\Delta_1$  and  $\Delta_2$ :

$$Q = \int D\{f, \chi, \Delta\} \exp \left\{ \int_0^{1/T} d\tau [S_0(\tau) + S_{\text{int}}(\tau)] \right\}, \quad (5)$$

where

$$S_0 = \sum_{k\sigma} c_{k\sigma}^+ \left( \frac{\partial}{\partial \tau} - \xi_k \right) c_{k\sigma} + f_i^+ \frac{\partial}{\partial \tau} f_i + \frac{1}{2} \chi_i \frac{\partial}{\partial \tau} \chi_i - \frac{1}{J} (|\Delta_1|^2 + |\Delta_2|^2), \quad (6)$$

$$S_{\text{int}} = (\Delta_1^* a_i + \Delta_2^* b_i) + \text{H.c.} \quad (7)$$

The structure (3) of the operators  $a_i$  and  $b_i$  implies that the coupling fields  $\Delta_1$  and  $\Delta_2$  describe correlations between localized states and conduction electrons in the particle–hole channel (the "excitonic" channel) and the "Cooper" particle–particle channel, respectively.

The ordinary pseudofermion representation of spin introduces a local gauge symmetry  $U(1)$ , and the phase of the coupling field  $\Delta$  can be removed by transforming the pseudofermion phase ("radial" gauge<sup>3</sup>). The Mattis representation (2) does not exhibit such continuous symmetry: the phases of the Fermi fields in (2) can be changed only by  $\pm\pi$ . In the given case we can pass to a "radial" gauge via the following global transformation, which incorporates electron fields as well:

$$f \Rightarrow f \exp(i\varphi_2 - i\varphi_1),$$

$$c_\uparrow(r) \Rightarrow c_\uparrow(r) \exp(i\varphi_2), \quad c_\downarrow(r) \Rightarrow c_\downarrow(r) \exp(i\varphi_1), \quad (8)$$

where  $\varphi_1$  and  $\varphi_2$  are the phases of the parameters  $\Delta_1$  and  $\Delta_2$  in (7), respectively. Note that in the single-impurity case considered the parameters  $\Delta$  and their phases are determined only at the site  $R_i=0$  occupied by a localized spin; at the same time, the transformation (8) is global and, hence, retains the form of the kinetic energy.

Substitution of (8) into (6) and (7) yields the following expression for the action:

$$S = S_0 + |\Delta_1|(a_i + a_i^\dagger) + |\Delta_2|(b_i + b_i^\dagger) + i\dot{\varphi}_-(S_i^z + \sigma^z) + \frac{1}{2}i\dot{\varphi}_+ n, \quad (9)$$

where  $S_0$  is given by (6), and  $a_i$  and  $b_i$  are defined in (3). In Eq. (9),  $\varphi_\pm = \varphi_1 \pm \varphi_2$  and

$$\sigma^z = \int d^3R \sigma^z(R), \quad n = \int d^3R n(R) \quad (10)$$

are, respectively, the total spin and the charge of the electron subsystem. The last two terms on the right-hand side of (9) reflect the fact that the total spin of the system and the number of current carriers are integrals of motion.

We distinguish the static ( $r_0$ ) and fluctuating ( $\delta r$ ) parts of the coupling parameters:

$$|\Delta_{1,2}| = r_0 + \delta r_{1,2}. \quad (11)$$

We restrict our discussion to the static approximation. The effective hybridization parameter  $r_0$  is found from the equation for the saddle point in the integral (5):

$$r_0 = \frac{1}{2} J \operatorname{Re} \langle a_i + b_i \rangle. \quad (12)$$

Allowing for the fact that  $\langle a_i \rangle = \langle b_i \rangle$ , we get

$$r_0 = \frac{J}{\sqrt{2}} \left\langle f_i^\dagger c_{i\uparrow} + \frac{\chi_i c_{i\downarrow}}{\sqrt{2}} \right\rangle. \quad (13)$$

In the approximation adopted here, where the fluctuations of  $\delta r$  and  $\varphi$  are not considered, the action (9) becomes a quadratic form and the averages in (13) are given by the following formulas:

$$\langle f_i^\dagger c_{i\uparrow} \rangle = -\frac{r_0}{\sqrt{2}} T \sum_\varepsilon F_\varepsilon G_\varepsilon, \quad (14)$$

$$\langle \chi_i c_{i\downarrow} \rangle = \frac{1}{\sqrt{2}} \langle f_i^\dagger c_{i\uparrow} \rangle.$$

Here the function

$$F_\varepsilon = -\langle T_\pi f_i f_i^\dagger \rangle_\varepsilon = (i\varepsilon + i\omega_k \operatorname{sgn} \varepsilon)^{-1}, \quad \omega_k = \pi \rho r_0^2, \quad (15)$$

is the pseudofermion Matsubara Green's function, and

$$G_\varepsilon = \sum_k G_{\varepsilon k}^0 \simeq -i\pi \rho \operatorname{sgn} \varepsilon, \quad |\varepsilon| < D, \quad (16)$$

is the initial single-site electron Green's function, with  $D$  the halfwidth of the conduction band. The energy  $\omega_k$  in (15) has the meaning of the frequency of the localized-spin Kondo fluctuations. Substituting (14) into (13), we arrive at an equation for determining  $\omega_k$ :

$$1 = -\frac{3}{4} J T \sum_\varepsilon F_\varepsilon G_\varepsilon. \quad (17)$$

For  $T \ll \omega_k$  this yields

$$\omega_k = D \exp\left(-\frac{4}{3\lambda}\right), \quad \lambda = J\rho. \quad (18)$$

The extra factor of  $\frac{3}{4}$  in (17) and (18) is a consequence of the mean-field approximation. It plays no essential role qualitatively and can be removed by allowing for the lowest-order fluctuation corrections in  $\delta r$  when calculating the averages in (13).

The impurity contribution to the dynamic spin susceptibility is (in Matsubara frequencies)

$$\chi_i(\omega) = -T \sum_\varepsilon F_\varepsilon F_{\varepsilon+\omega} = \frac{2\omega_k}{\pi|\omega|(|\omega| + 2\omega_k)} \times \left\{ \psi\left(\frac{1}{2} + \frac{\omega_k + |\omega|}{2\pi T}\right) - \psi\left(\frac{1}{2} + \frac{\omega_k}{2\pi T}\right) \right\} \simeq \frac{1}{\pi(|\omega| + \omega_k)} \quad \text{if } |\omega|, \quad T < \omega_k. \quad (19)$$

Here  $\psi$  is the logarithmic derivative of the gamma function (the digamma function). The static spin susceptibility is

$$\chi_i = \frac{1}{2\pi^2 T} \psi'\left(\frac{1}{2} + \frac{\omega_k}{2\pi T}\right) \simeq \begin{cases} (\pi\omega_k)^{-1} & \text{if } T \ll \omega_k, \\ (4T)^{-1} & \text{if } T \gg \omega_k, \end{cases} \quad (20)$$

where  $\psi'$  is the trigamma function. Formulas (19) and (20) correspond to the well-known expressions for the susceptibility of a Kondo impurity (see, e.g., Ref. 29). Note that since the representation (2) introduces no unphysical spin-zero states, for  $T \gg \omega_k$  the expression (20) yields the correct value of the Curie constant. For  $T \ll \omega_k$  Eqs. (19) and (20) yield Korringa's Fermi liquid relation:

$$\left(\frac{\chi_i''(\omega)}{\omega}\right)_{\omega \rightarrow 0} = \pi \chi_i^2. \quad (21)$$

The contribution of spin excitations to the specific heat for  $T \ll \omega_k$  also has the Fermi liquid form  $C_i = \gamma_s T$ , where the constant  $\gamma_s$  is determined by the spectral density of  $f$ - and  $\chi$ -fermions:

$$\gamma_s = \gamma^f + \gamma^x = \frac{3}{2} \gamma^f = \frac{\pi^2}{2} \rho^f = \frac{\pi}{2\omega_k}. \quad (22)$$

The numerical factor in (22) can be explained by the fact that the entropy related to the real field  $\chi$  is only half the entropy of ordinary  $f$ -fermions. Here the Wilson ratio is

$$R = \frac{\pi^2}{S(S+1)} \left( \frac{\chi_i}{\chi_s} \right) = \frac{8}{3}. \quad (23)$$

This relation gives the value of  $R$  found by Coleman *et al.*,<sup>15</sup> which is somewhat higher than the exact value of 2. The Fermi liquid behavior of the Kondo impurity at low temperatures is, as is well known, a consequence of the screening of localized-spin excitations by the low-frequency electron spin density fluctuations. The nature of the distribution of the compensating spin density near the impurity is determined by the dependence of the correlator  $\langle S_\tau(0)\sigma_{\tau'}(R) \rangle$  on distance. In the limit  $\tau' \rightarrow \tau$ , the mean-field approximation yields

$$\begin{aligned} \langle S_\tau^z(0)\sigma_\tau^z(R) \rangle &= |\langle f_i^+ c_\tau(R) \rangle|^2 \\ &= -\frac{r_0^2}{2} \left| T \sum_\varepsilon F_\varepsilon F_\varepsilon^0(R) \right|^2. \end{aligned} \quad (24)$$

If we allow for the fact that for  $k_0 R > 1$  ( $k_0$  is the Fermi momentum) the electron Green's function is

$$G_\varepsilon^0(R) = -\frac{\pi\rho}{k_0 R} \exp\left\{ ik_0 R \operatorname{sgn} \varepsilon - \frac{|\varepsilon|R}{v_f} \right\}, \quad (25)$$

where  $v_f$  is the Fermi velocity, Eq. (24) yields

$$\langle S_\tau^z(0)\sigma_\tau^z(R) \rangle = -\frac{\omega_k}{2\pi} \left( \frac{\sin k_0 R}{k_0 R} \right)^2 f^2 \left( \frac{R}{R_k} \right),$$

$$f(x) = -e^x \operatorname{Ei}(x)$$

$$\approx \begin{cases} -\ln \gamma x & \text{if } x \ll 1, \\ x^{-1} & \text{if } x \gg 1. \end{cases} \quad (26)$$

Here  $\operatorname{Ei}(-x)$  is the exponential integral function, and  $\gamma$  is Euler's constant. The radius  $R_k = v_f/\omega_k$  determines the characteristic size of the Kondo complex formed because of resonance scattering of electrons on the impurity. The integral of (26) over the volume (the result is equal to  $-\frac{1}{2}$ ) is independent of the coupling constant  $\lambda$  and is determined by distances  $R \lesssim R_k$ . Except for unessential details, the formula (26) coincides with the one derived by Millis and Lee.<sup>6</sup>

For further discussion it is essential to examine the behavior of Green's function

$$K_\omega(R) = \langle T_\tau S^z(0)\sigma^z(R) \rangle_\omega \quad (27)$$

at low frequencies. In the loose binding limit  $T \gg \omega_k$ ,

$$K_\omega(R) = \chi_p \chi_i(\omega) \frac{J}{4\pi R^3} \cos 2k_0 R, \quad (28)$$

where  $\chi_p = \rho/2$  is the Pauli susceptibility, and  $\chi_i(\omega) = \chi_i \delta_{\omega,0}$  the susceptibility of the free impurity spin. Here and in what follows we assume  $k_0 R > 1$ . This standard expression for RKKY polarization is a consequence of the purely elastic scattering of an electron at an impurity, with an

amplitude  $J$  independent of the electron energy. As the temperature decreases, the effective amplitude  $J_{\text{eff}}$  for low-energy electrons begins to grow, as is well known, and this leads to a change in polarization over large distances. In the tight binding limit  $T \ll \omega_k$  we ignore the fluctuations in  $\Delta$  and  $\varphi$  in (9) and get

$$\begin{aligned} K_\omega(R) &= -\frac{r_0^2}{2} T \sum_\varepsilon F_\varepsilon F_{\varepsilon+\omega} G_\varepsilon^0(R) G_{\varepsilon+\omega}^0(R) \\ &= \chi_p \frac{e^{-y}}{(k_0 R)^2} \left\{ \cos(2k_0 R) \frac{\omega_k}{|\omega|} \right. \\ &\quad \times [e^{2y} \operatorname{Ei}(-x-2y) - \operatorname{Ei}(-x)] e^x \\ &\quad \left. - \frac{\ln(1+|\omega|/\omega_k)}{2+|\omega|/\omega_k} \right\}, \end{aligned} \quad (29)$$

where

$$x = \frac{2R}{R_k}, \quad y = \frac{R|\omega|}{v_f}.$$

Let us examine the behavior of the correlator (29) in the limiting cases. In the static limit we have  $\omega=0$  and for arbitrary values of  $R$

$$K_0(R) = \chi_p \chi_i \frac{1}{\rho 4\pi R^3} \cos(2k_0 R) \phi \left( \frac{2R}{R_k} \right), \quad (30)$$

where

$$\begin{aligned} \phi(x) &= x + x^2 e^x \operatorname{Ei}(-x) \\ &\approx \begin{cases} 1 & \text{if } x \gg 1, \\ x & \text{if } x \ll 1. \end{cases} \end{aligned} \quad (31)$$

At large distances  $R > R_k$  the greatest contribution to (30) is provided by electrons with low energies  $\xi < \omega_k$ . Comparing (30) for  $R \gg R_k$  with the appropriate high-temperature expression (28) for  $\phi=1$ , we see that they coincide if the exchange integral in (26) is replaced by the effective value  $J_{\text{eff}} = \rho^{-1}$ . At small distances there is, naturally, no such enhancement because polarization occurs owing to high-energy electrons. Indeed, if in (30) we put  $R \sim a \sim \pi/k_0$ , we find that (30) yields a quantity  $2\pi\omega_k/J$  times smaller than (28) does. This is understandable because Eq. (30) does not account for high-energy processes (fluctuations of the coupling parameters  $\Delta(\tau)$ ). Actually, RKKY polarization does not change substantially over distances on the order of the lattice constant, with the exception of renormalization of roughly  $\lambda \ln \lambda$ , as noted by Cox.<sup>22</sup>

At low frequencies  $\omega < \omega_k$  and for  $R > R_k$  Eq. (29) yields

$$\begin{aligned} K_\omega(R) &= \chi_p \chi_i(\omega) \frac{1}{\rho 4\pi R^3} \left( \cos(2k_0 R) - \frac{R|\omega|}{v_f} \right) \\ &\quad \times \exp \left\{ -\frac{R|\omega|}{v_f} \right\}, \end{aligned} \quad (32)$$

with the dynamic susceptibility  $\chi_i(\omega)$  specified in (19). We see that (32) corresponds exactly to the spin polarization that arises because of exchange scattering of electrons at a localized level with a susceptibility  $\chi_i(\omega)$ , with a scattering am-

plitude  $J_{\text{eff}} = \rho^{-1}$ . This result finds a natural interpretation in the theory of Nozieres.<sup>20</sup> As long as we are interested in large distances  $R > R_k$ , the Kondo complex acts as a point-like formation. The effective interaction of electrons with the Kondo complex is concentrated primarily at low frequencies  $\omega \ll \omega_k$ ; hence the local electron–electron interaction via the impurity polarization, whose value is

$$V_{e-c}(\xi, \xi' \ll \omega_k) = J_{\text{eff}}^2 \chi_x(\omega) \approx \frac{1}{\pi \omega_k \rho^2}, \quad (33)$$

is highly retarded. The quantity specified by (33) corresponds to the electron–electron scattering amplitude  $A$  introduced by Nozieres<sup>20</sup> and also calculated by Lee.<sup>30</sup>

The fact that the effective amplitude of the interaction of the electrons on the Fermi surface with Kondo-singlet excitations has the scale  $\rho^{-1}$  follows readily from (29). Let us define this amplitude in terms of the three-point Green's function

$$\langle S_{\omega}^z(i) c_{\varepsilon, \sigma}(R) c_{\varepsilon + \omega, \sigma}^+(R') \rangle = \frac{1}{2} \langle S_i^z S_i^z \rangle_{\omega} J_{\text{eff}}(\varepsilon, \varepsilon + \omega) \times G_{\varepsilon}^0(R) G_{\varepsilon + \omega}^0(R'). \quad (34)$$

The function  $K_{\omega}(R)$  of (27) is obtained by summing (34) with respect to energy  $\varepsilon$  at  $R = R'$ . At the same time, while  $\omega < \omega_k$  and  $R > R_k$  hold, this function is essentially determined by the mean-field expression (29), with the main dependence on  $\varepsilon$  in (29) contained in the electron Green's functions, since the local functions  $F_{\varepsilon}$  defined in (15) contain the “massive” term  $\omega_k$ . Comparing now the expressions (29) and (34), we note that the amplitude of the interaction between an electron and spin fluctuations at low energies is

$$J_{\text{eff}}(|\varepsilon|, |\varepsilon + \omega| \ll \omega_k) \approx -\frac{r_0^2 F_{\varepsilon}^2}{\chi_i} \approx \frac{1}{\rho}. \quad (35)$$

### 3. “HEAVY” FERMIONS IN A PERIODIC LATTICE

As noted in the Introduction, our discussion of low-energy electronic states in the Kondo lattice is based on the view expressed by some researchers that the “heavy” charged Fermi liquid is the result of renormalization of an ordinary band caused by the interaction of dynamic spin fluctuations and Kondo centers, whose spectrum in the low-frequency limit  $\omega \leq \omega_k$  is, as we saw earlier, of a localized Fermi liquid nature. The analysis done in Sec. 2 suggests that the effective value of the interaction between low-energy electrons and spin fluctuations has the scale  $\rho^{-1}$ . As for the spin Green's function, in the lattice it obviously differs from that given by Eq. (15) because of the effect of the spin–spin RKKY interaction. In this section, however, we ignore the RKKY exchange effects, having in mind the range of values of parameter  $J$  where  $E(\text{RKKY}) \ll \omega_k$ .

According to what has just been said, the self-energy of a conduction electron in the Born approximation has the form (in Matsubara frequencies):

$$\Sigma(i\varepsilon, k) = \frac{3}{4} T \sum_{\omega, q} J_{\text{eff}}^2(\varepsilon, \varepsilon + \omega) \chi(\omega) G_{\varepsilon + \omega}(k + q). \quad (36)$$

Using Eqs. (19) and (35) for  $\chi(\omega)$  and  $J_{\text{eff}}$ , respectively, we arrive at the following expression for the self-energy at  $T = 0$ :

$$\Sigma(i\varepsilon) = -i \operatorname{sgn}(\varepsilon) \frac{3}{4\pi\rho} \ln\left(1 + \frac{|\varepsilon|}{\omega_k}\right). \quad (37)$$

This expression is valid for  $\varepsilon < \omega_k$ . It implies that

$$\Sigma'(\omega) = -\frac{\omega}{Z_0}, \quad \Sigma''(\omega) = -\frac{\omega^2}{Z_0 2\omega_k}, \quad (38)$$

where the renormalization constant (the quasiparticle weight)  $Z_0$  is specified by the following relation:

$$Z_0 = \frac{4\pi}{3} \rho \omega_k. \quad (39)$$

Formulas (38) and (39) suggest that for  $T \ll \omega_k$  quasiparticle states are formed near the Fermi surface in a region whose width is of order  $\omega_k$ . In this region the retarded Green's function of the current carriers is determined primarily by its pole part,

$$G^R(\omega, k) = \frac{Z_0}{\omega - \tilde{\xi}_k + i\gamma_k(\omega)}. \quad (40)$$

Here  $\tilde{\xi}_k = Z_0 \xi_k$  is the energy of a quasiparticle with an effective mass  $M^*$  greater than the initial mass  $m$  by a factor  $Z_0^{-1}$ . The damping of this “heavy” current carrier,

$$\gamma_k(\omega) = \frac{\omega^2}{2\omega_k}, \quad (41)$$

has the Fermi liquid form. Equations (38) and (41) cause the resistivity to have a quadratic temperature dependence, which reaches the unitary limit at temperatures of the order of  $T_k$ .

Obviously, quasiparticle excitations in the Kondo lattice also occur at extremely high energies,  $\omega \gg \omega_k$ , where their spectrum can be calculated using perturbation-theory techniques. However, within a broad range from energies of the order of  $\omega_k$  to energies  $\tilde{\omega}$ , the motion of current carriers is completely incoherent. This incoherent part of the current-carrier spectral density apparently corresponds to the electron component of a multiparticle Kondo resonance. The energy  $\tilde{\omega}$  can be estimated from the equation

$$\tilde{\omega} = \frac{1}{\rho \ln^2(\tilde{\omega}/\omega_k)}, \quad (42)$$

where the right-hand side is, in the logarithmic approximation, an estimate of the relaxation rate of electrons whose energy is  $\tilde{\omega}$  in the Kondo lattice.

In the present approximation the electron self-energy is momentum-independent and the shape of the Fermi surface does not change, but, of course, it can be distorted to a certain extent by the emerging spatial dispersion of spin excitations due to spin–spin interaction.

The higher density of states  $\tilde{\rho} = \rho/Z_0$  in the quasiparticle band near the Fermi level leads to an enhanced constant in the linear part of specific heat for  $T < \omega_k$ :

$$\gamma_e = \frac{2\pi^2}{3} \tilde{\rho} = \frac{\pi}{2\omega_k}. \quad (43)$$

The current-carrier contribution  $\gamma_e$  established by (43) has the same value as the localized Fermi liquid contribution  $\gamma_s$  given by (22), related to the excitation of  $f$ - and  $\chi$ -pseudofermions and having a purely spin nature. Bearing in mind that for  $E(\text{RKKY}) \ll \omega_k$  the localized "spin" liquid does not undergo any substantial changes, we arrive at the following expression for the total specific heat:

$$\gamma = \gamma_s + \gamma_e = \frac{\pi}{\omega_k}. \quad (44)$$

As for the spin susceptibility of current carriers, it does not undergo much renormalization, in contrast to the entropy. The point is that the high density of states  $\tilde{\rho}$  in the "heavy" conduction band is exactly balanced by the smallness of the quasiparticle weight  $Z_0$  in the electron wave function. For one thing, the quantity

$$\begin{aligned} \frac{\chi_e''(\omega)}{\omega} &= \frac{\pi}{4} \int \frac{d\omega}{2T \cosh^2(\omega/2T)} \left[ \frac{1}{\pi} \text{Im} \sum_k G^R(\omega, k) \right]^2 \\ &= \frac{\pi}{2} (Z_0 \tilde{\rho})^2 = \frac{\pi}{2} \rho^2, \end{aligned} \quad (45)$$

which determines the contribution of the conduction band to the rate of the Korringa relaxation of nuclei, remains unrenormalized. Such a compensation effect explains why when conduction electrons constitute the dominant channel in the relaxation of test magnetic moments there can be no "heavy-fermion" effects.<sup>31,18</sup> More typical, from the experimental viewpoint, is the situation where relaxation in the fluctuations of the localized spin of a rare-earth ion is dominates. For  $T < \omega_k$  this channel also yields a linear temperature dependence, imitating enhanced Korringa relaxation:

$$T_1^{-1} = 2\pi(A\chi_i)^2 T = \frac{2}{\pi} \left( \frac{A}{\omega_k} \right)^2 T. \quad (46)$$

Here we have used Korringa's relation (21), and  $A$  is the coupling constant in the interaction of a test nuclear (electron) moment with the spin of a rare-earth ion. If we allow for (44), the Wilson ratio in the lattice becomes close to unity:  $R = \frac{4}{3}$ .

Thus, for the Kondo lattice at low temperatures we have the two-liquid picture: one liquid, almost localized, determines the spin response, and the other, the renormalized conduction band, is responsible for phenomena related to charge transfer. Such a picture was discussed in detail by Kagan *et al.*,<sup>7,32</sup> but, in contrast to those researchers, it was found that both components contribute equally to the thermodynamics of the problem and that the low-energy behavior is characterized by a single energy scale  $\omega_k$ . The same energy scale determines the magnitude of the residual interaction between "heavy" quasiparticles at the Fermi level, which can be estimated by multiplying the strength of the interaction between electrons [Eq. (33)] by the square of the wavefunction renormalization factor  $Z_0$ .

Such universal behavior is partially the result of our use of the impurity expression for the spin fluctuations correlator on the assumption that the RKKY interaction is much lower than the frequency of Kondo fluctuations. In Sec. 4 we show that for  $E(\text{RKKY}) \sim \omega_k$ , a new energy scale appears that disrupts the single-parameter behavior.

#### 4. THE COHERENCE TEMPERATURE IN THE KONDO LATTICE

The goal of this section is to establish how the renormalization of electronic states changes if we consider the correlation between spins caused by the RKKY interaction. The RKKY energy scale is basically determined by the interaction at small distances on the order of the lattice constant. At such distances the RKKY polarization forms owing to high-energy electrons and, as noted earlier, experiences no sizable renormalizations. Hence, we assume that the potential  $J_H(R)$  of the Heisenberg interaction

$$H(\text{RKKY}) = - \sum_{\langle ij \rangle} J_H(R_{ij}) (S_i S_j) \quad (47)$$

is a free parameter, which theoretically can be calculated via perturbation-theory techniques as the initial RKKY integral plus logarithmic Kondo corrections. In essence, the smallness of the renormalization of the RKKY interaction is one of the main reasons for the nonuniversal behavior of real Kondo systems at low temperatures, systems that manifest a multitude of magnetic and electronic properties. If we allow for (47), we are dealing with the Kondo-Heisenberg model, often used to describe heavy-fermion systems (see, e.g., Ref. 33).

Let  $J_q$  be the Fourier transform of the RKKY integral. In the random phase approximation (RPA) we have the following expression for the dynamic spin susceptibility:

$$\chi_q(\omega) = \frac{\chi_i(\omega)}{1 - J_q \chi_i(\omega)}, \quad (48)$$

where  $\chi_i(\omega)$  is the single-site susceptibility, for which we use Eq. (19). Equation (48) takes into account the spin-spin correlations in the lattice in the simplest possible way. Of course, the RPA is insufficient near a magnetic instability proper, that is, when a pole appears in the expression (48) for spin-wave excitations. When spin correlations are well-developed, the problem must be solved by applying Moriya's self-consistent theory,<sup>34</sup> allowing for the effect of these correlations on the single-ion susceptibility  $\chi_i(\omega)$  via the renormalization of the pseudofermion functions  $F$  [see Eq. (15)]. Here we restrict our discussion to a qualitative picture of the situation in the RPA. This leads to the expression

$$\chi_q(\omega) = \frac{1}{\pi(\omega_k - i\omega - J_q/\pi)}, \quad (49)$$

which can also be written as<sup>35</sup>

$$\chi_q(\omega) = \chi_q \frac{i\Gamma_q}{\omega + i\Gamma_q}, \quad (50)$$

where

$$\chi_q = \frac{1}{\pi\omega_k - J_q} \quad (51)$$

is the wave-vector dependent static susceptibility, and  $\Gamma_q = (\pi\chi_q)^{-1}$  is the damping factor. If  $J_q$  reaches its peak value at  $q=Q$ , near  $Q$  the susceptibility assumes the form

$$\chi_{Q+q}(\omega) \approx \frac{1}{\pi(\omega_{sf} - i\omega + D_s q^2)}, \quad (52)$$

$$\omega_{sf} = \omega_k(1 - J_Q \chi_i) \approx \omega_k - \frac{J_Q}{\pi}, \quad D_s = \frac{J_Q - J_{Q+q}}{\pi q^2}.$$

The quantity  $D_s$  depends on the type of lattice and the form of the function  $J_H(R)$ ; roughly, its scale is determined by the value of the exchange integral over the lattice constant:  $D_s \sim J_H(a)a^2$ . Equation (52) implies that  $\sqrt{D_s/\omega_{sf}} = \xi_m$  determines the spin correlation length. Note that since the single-site susceptibility  $\chi_i$  in the expression for frequency  $\omega_{sf}$  is temperature-dependent [according to Eq. (20),  $\chi(T) \sim \chi(0)(1 - \pi^2 T^2/3\omega_k^2)$  for  $T \ll \omega_k$ ], the length  $\xi_m$  decreases as the temperature grows.

The chief meaning of Eq. (52) is that when the RKKY energy begins to compete with  $\pi\omega_k$ , a relaxation mode appears that has an energy  $\omega_{sf} \ll \omega_k$  in a narrow region of the Brillouin zone near the vector  $Q$  of the expected magnetic ordering. Such (anti)ferromagnetic paramagnon excitations are characteristic for strongly correlated systems with short-range spin order and are being actively discussed, for one thing, in connection with high- $T_c$  superconductivity (see, e.g., Refs. 36 and 37). The role that paramagnons play in the thermodynamics of heavy-fermion systems was studied by Ohkawa.<sup>23</sup>

Let us now examine the effect of spin-spin correlations on the self-energy of conduction electrons by employing the spin susceptibility in (36) in the form (52). Again assuming that  $J_{\text{eff}} = \rho^{-1}$  in the low-energy limit and performing standard transformations, we find that

$$\Sigma(\omega + i\delta, k) = -\frac{3}{8\pi\rho^2} \sum_q \int dx \chi''_{Q+q}(x) \times \frac{\tanh(\chi'/2T) - \coth(x/2T)}{\omega + x - \xi' + i\delta}, \quad (53)$$

where  $\chi''(x)$  is the imaginary part of the susceptibility (52), and  $\xi' = \xi(k+Q+q)$ . At low temperatures,

$$Z_0 \Sigma''(\omega, k) = -\frac{\pi\omega_k}{\rho} \sum_q \chi''_{Q+q}(\omega - \xi') \theta(\xi') \theta(\omega - \xi'), \quad (54)$$

$$Z_0 \Sigma'(\omega, k) = -\frac{2\omega\omega_k}{\rho} \sum_q \int_0^\infty dx \frac{\chi''_{Q+q}(x) \theta(\xi')}{(x + \xi')^2 - \omega^2}, \quad (55)$$

where  $\theta$  is the Heaviside unit function, and the constant  $Z_0$  is defined in (39). The paramagnon contribution (small values of  $q$ ) is important only if the scattered-electron momentum  $k' = k + Q + q$  is near the Fermi surface and  $\xi' < \omega_k$ . This is possible in two cases: when vector  $Q$  is zero (ferromagnetic correlations between spins), and when  $Q$  coincides in magnitude with the diameter  $2k_0$  of the cross section of the

Fermi sphere (for simplicity we consider only the completely isotropic case). The situation when  $Q \sim 2k_0$  holds is quite typical of rare-earth compounds, where RKKY exchange is a source of helical magnetic structures. Moreover, for purposes of qualitative analysis we assume that  $Q$  is equal either to 0 or to  $2k_0$ .

In both cases, passing in (54) and (55) from the sum over momenta to integration with respect to the variables  $\xi'$  and  $y = \frac{1}{2}(1 - \cos \vartheta)$ , where  $\vartheta$  is the angle between  $k'$  and  $k+Q$ , we get

$$Z_0 \Sigma''(\omega) = -\omega_k \int_0^\omega d\xi' \xi' \int_0^1 \frac{dy}{\xi'^2 + (\omega_{sf} + 4D_s k_0^2 y)^2} \approx -\frac{\omega_k}{4D_s k_0^2} \left\{ \omega \cot^{-1} \left( \frac{\omega_{sf}}{\omega} \right) - \frac{\omega_{sf}}{2} \ln \left( 1 + \frac{\omega^2}{\omega_{sf}^2} \right) - \frac{\omega^2}{2(\omega_{sf} + 4D_s k_0^2)} \right\}. \quad (56)$$

When  $E(\text{RKKY})$  is low, that is,  $D_s \rightarrow 0$  and  $\omega_{sf} \rightarrow \omega_k$ , Eq. (56) yields the result (38) for  $\Sigma''(\omega)$ , determined by inelastic scattering at localized Kondo fluctuations. But if the RKKY interaction is fairly strong, so that  $D_s(2k_0)^2 \sim \omega_k \gg \omega_{sf}$ , the damping is quadratic in  $\omega$  only at frequencies  $\omega < \omega_{sf}$ :

$$Z_0 \Sigma''(\omega) \approx \begin{cases} -\frac{\omega^2}{2\omega_{sf}} & \text{if } \omega < \omega_{sf}, \\ -\frac{\pi\omega}{2} & \text{if } \omega_{sf} < \omega < \omega_k. \end{cases} \quad (57)$$

Thus, the presence of low-frequency (anti)ferromagnetic paramagnons caused by RKKY correlations "delays" the transition of the Kondo lattice to the Fermi liquid mode. Strictly speaking, in the frequency range  $\omega_{sf} < \omega < \omega_k$ , or in the temperature range  $\omega_{sf} < T < \omega_k$ , no quasiparticles participate in the process, since their damping is on the order of their energy. It is natural to identify the crossover temperature  $T_{\text{cr}} \sim \omega_{sf}$  with the coherence temperature  $T_{\text{coh}} < T_k$  of heavy-fermion systems, introduced empirically as the temperature of a smooth transition to the Fermi liquid mode. For one thing, relation (57) signifies a transition from a linear temperature dependence of the resistivity to a quadratic dependence at temperatures on the order of  $\omega_{sf}$ . The magnitude of  $\omega_{sf}$  proper depends, according to (52), on the closeness of the system to magnetic disorder. Note, however, that although the results specified by Eqs. (56) and (57) are common for ferromagnetic and antiferromagnetic correlations, the relaxation transport time and resistivity are sensitive to the paramagnon effect only in the second case, while in the first only forward scattering ( $Q=0$ ) is enhanced. Note also that the linear dependence of resistivity in systems with antiferromagnetic correlations has been repeatedly discussed in the context of high- $T_c$  superconductivity, starting with the work of Moriya *et al.*<sup>36</sup>

The real part of the self-energy, Eq. (55), is

$$Z_0 \Sigma'(\omega) = -\frac{2\omega}{\pi} \int_0^\infty d\xi' dx \frac{x}{(x+\xi')^2 - \omega^2} \times \int_0^1 \frac{dy \omega_k}{\xi'^2 + (\omega_{sf} + 4D_s k_0^2 y)^2}. \quad (58)$$

At low frequencies  $\omega < \omega_{sf}$  this becomes

$$Z_0 \Sigma'(\omega) = -\frac{\omega \omega_k}{4D_s k_0^2} \ln \left( 1 + \frac{4D_s k_0^2}{\omega_{sf}} \right), \quad (59)$$

which again yields (38) when  $D_s$  is sent to zero. In the presence of fairly strong spin-spin correlations, when  $D_s(2k_0)^2 \sim \omega_k \gg \omega_{sf}$ , Eq. (59) predicts an additional decrease in the quasiparticle weight:

$$Z_0' \approx \frac{Z_0}{\ln(4D_s k_0^2 \omega_{sf})}. \quad (60)$$

In the intermediate frequency range  $\omega_{sf} < \omega < \omega_k$ ,

$$Z_0 \Sigma'(\omega) \approx -\omega \ln \left( \frac{4D_s k_0^2}{\omega} \right), \quad (61)$$

which corresponds to the already noted "marginal behavior" of quasiparticles with an energy  $\omega > \omega_{sf}$ .

The (anti)ferromagnetic fluctuations discussed also affect, for instance, the nuclear spin relaxation rate, which is proportional to  $\chi''(\omega)/\omega$ . For  $T < \omega_k$  and within the RPA, instead of (21) we arrive at (as  $\omega \rightarrow 0$ )

$$\frac{\chi''(\omega)}{\omega} = \pi \sum_q \frac{1}{(\chi_i^{-1}(T) - J_q)^2} \approx \frac{1}{\pi} \sum_q \frac{1}{(\omega_{sf}(T) + D_s q^2)^2} = \frac{a^3}{8\pi^2 D_s^2} \xi_m(T), \quad (62)$$

where  $\xi_m(T) = \sqrt{D_s/\omega_{sf}(T)}$  is the magnetic correlation length. The temperature dependence of  $\omega_{sf}$  is determined by the susceptibility  $\chi_i(T)$  from Eq. (20). Using its expansion and assuming that  $\omega_{sf} \ll \omega_k$ , we find that

$$\omega_{sf}(T) \approx \omega_{sf}(0) \left( 1 + \frac{1}{3} \frac{\pi^2 T^2}{\omega_{sf} \omega_k} \right). \quad (63)$$

By combining (62) and (63), we can express the temperature dependence of the nuclear relaxation rate for  $T < \omega_k$  as

$$T_1^{-1} \sim T \xi_m(T) \sim T \left( 1 + \frac{1}{3} \frac{\pi^2 T^2}{\omega_{sf} \omega_k} \right)^{-1/2}. \quad (64)$$

Note that the numerical factor of  $\frac{1}{3}$  in (63) and, hence, in (64) is actually understated; if the temperature dependence of the Kondo fluctuations frequency<sup>29</sup> is also considered, the factor becomes equal to  $\frac{2}{3}$ . Moreover, as noted earlier, paramagnon effects also renormalize  $\chi_i(T)$  in a self-consistent manner.<sup>34</sup> Nevertheless, the approximation (64) clearly shows that the linear Korringa dependence is reached only at temperatures much lower than  $\omega_k$  and that the nature of the relaxation is controlled by two parameters,  $\omega_k$  and  $\omega_{sf}$ .

Experimentally, the coherence temperature is also characterized by the peak spin susceptibility and the peak value of  $\gamma(T) = C(T)/T$ , which is usually interpreted as proof that

a local minimum has emerged in the density of states of the Kondo resonance near the Fermi level.<sup>38</sup> Such a pseudogap in the spectrum of localized pseudofermions ("spinons") might have emerged if we had carefully considered the effect of short-range spin order on the one-particle Green's functions of the  $f$ - and  $\chi$ -fermions in the lattice. Of course, the RPA does not have the capacity to allow for short-range magnetic order, which is, obviously, also a source of inelastic neutron scattering at low temperatures.<sup>27</sup>

Equation (52) acquires a pole provided that  $J_Q = \pi \omega_k$ , which must be assumed identical to the Doniach condition.<sup>39</sup> For  $J_Q > J_Q^c = \pi \omega_k$  we have the ordered phase, in which the magnetic moment per site is determined in the molecular field approximation by the self-consistency equation

$$m = 2 \langle f_i^+ f_i^- - \frac{1}{2} \rangle = 2T \sum_\varepsilon \frac{1}{i\varepsilon + i\omega_k \operatorname{sgn} \varepsilon + J_Q m/2} = \frac{2}{\pi} \tan^{-1} \left( \frac{\pi J_Q m}{2J_Q^c} \right). \quad (65)$$

The quantity  $\frac{1}{2} J_Q m$  in (65) acts as a chemical potential for the  $f$ -fermion and determines the scale of the pseudogap in the spectrum of such fermions. Equation (65) in the magnetic moment  $m$  has a nonzero solution for  $J_Q \geq J_Q^c$ . Near the critical value,  $x = J_Q/J_Q^c \sim 1$ , the magnetic moment is suppressed because of Kondo fluctuations, with  $m \approx \sqrt{x-1}$ , as obtained earlier by Bredl *et al.*<sup>40</sup> and Cox.<sup>22</sup>

## 5. DISCUSSION OF RESULTS

Thus, building on the ideas of Varma<sup>18</sup> and Éliashberg,<sup>19</sup> we have shown that a "heavy" band of current carriers forms in the Kondo lattice as a result of the interaction of electrons and almost localized virtual spin fluctuations. We calculated the fluctuation spectrum in the single-site approximation<sup>21</sup> and allowed further for the spin-spin RKKY interaction in the RPA. As for the effective amplitude for scattering of Fermi-surface electrons by spin fluctuations, we found from analyzing the single-impurity problem that  $J_{\text{eff}} \sim 1/\rho$ . This aspect is important because it ensures universal behavior at low temperatures.

The appearance of quasiparticles at low temperatures in the given approach is a consequence of the fact that the Kondo interaction generates a finite energy of the localized spin fluctuations,  $\omega_k$ . Hence, inelastic electron scattering, which damps such fluctuations, is found to be "frozen" when both  $\omega$  and  $T$  are lower than  $\omega_k$ . At the same time, the fairly strong RKKY interaction decreases the spectral density of the spin excitations at low frequencies  $\omega_{sf}$  caused by (anti)ferromagnetic paramagnons. Hence, the Fermi liquid behavior of Kondo lattices that are close to magnetic ordering is expected only below temperatures  $T_{\text{coh}} \sim \omega_{sf}$ . The Fermi liquid is, apparently, retained also under moderate doping of the lattice with nonmagnetic ions, although here the current carriers will not have a definite quasimomentum because of strong (on the order of the unitary limit) elastic scattering on nonmagnetic carriers.

We found that the low-temperature entropy of the current-carrier "heavy" band is commensurate in magnitude



with the contribution of the localized “spinon” liquid, which, apparently, explains the size of the jump in specific heat when heavy-fermion systems transfer into the superconducting state. At the same time, the qualitative modification of the nature of the spin relaxation of nuclei strongly supports the idea of simultaneous transformation of the spin liquid. As a result, apparently, there appears a V-like pseudogap in the density of “spinon” excitations if the ordinary  $T_1^{-1} \propto T^3$ -law is taken into account (see Ref. 41). We can assume that there is probably pairing between “spinons” suitable energywise for landing in the region of the superconducting gap in the “heavy” band of the current carriers.

In the suggested theory, the case of a half-filled band,  $n_e = 1$ , is not represented by a singular point, as long, of course, as the initial constant  $\lambda = J\rho$  is much smaller than unity. (Note that we are dealing here only with the three-dimensional Kondo lattice, with a regular density of states at the Fermi level.) Apparently, the point  $n_e = 1$  is singular, corresponding to an insulator state, only in the Zhang–Rice limit  $\lambda \gg 1$ , where at each site there is a localized bound state of an “individual” electron and the spin. In this limit, the triplet sector as well as itinerant vacant states and doubly electron-occupied states are separated by a finite gap and are effectively absent from the picture, reducing the state basis. It is not obvious how this picture can be adiabatically transformed into the case where  $\lambda \ll 1$  holds, when formation of a low singlet-triplet energy  $\omega_k$  is essentially a collective effect. This paper has assumed that as long as  $\omega_k$  is much smaller than the bandwidth, the wave function of the conduction electrons near the Fermi surface has an extended nature (as extended as the quasiparticle weight is small) irrespective of  $n_e$  and that the topology of the Fermi surface does not change dramatically. At the same time, resonance scattering of electrons on localized states leads to a situation in which the greater part of the wave function has a localized (over distances on the order of  $R_k$ ) incoherent nature and participates in the formation of a multiparticle Kondo resonance. It is assumed here that for  $\lambda \ll 1$  the three-dimensional Kondo lattice is a metal even for  $n_e = 1$  since it has no exact nesting, which in low-dimensional systems is known to help the spectrum acquire features inherent in an insulator by enhancing the interaction of electrons and spin fluctuations at the edge of the Brillouin zone. The tricky question of the mutual correspondence of the two limits discussed here in the case of  $n_e = 1$  is closely linked to the problem posed by Noziers<sup>42</sup> concerning the insufficient number of electrons in the Kondo lattice and requires further investigation.

This paper can be considered a development of the semi-phenomenological theories of Varma<sup>18</sup> and Éliashberg.<sup>19</sup> The weakest point in it is the combination of the single-site approximation and the RPA. In this approach the interaction of the phases of the effective hybridization parameters  $\Delta_i$  at different sites is completely ignored.

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- <sup>1</sup> P. Fulde, J. Keller, and G. Zwirnagl, *Solid State Phys.* **41**, 1 (1988).
- <sup>2</sup> J. M. Lawrence and D. L. Mills, *Comments Condens. Mat. Phys.* **15**, 163 (1991).
- <sup>3</sup> N. Read and D. M. Newns, *J. Phys. C* **16**, 3273 (1983).
- <sup>4</sup> P. Coleman, *Phys. Rev. B* **29**, 3035 (1984); **35**, 5072 (1987).
- <sup>5</sup> A. Auerbach and K. Levin, *Phys. Rev. Lett.* **57**, 877 (1986).
- <sup>6</sup> A. J. Millis and P. A. Lee, *Phys. Rev. B* **35**, 3394 (1987).
- <sup>7</sup> Yu. Kagan, K. A. Kikoin, and N. V. Prokof'ev, *Physica B* **182**, 201 (1992).
- <sup>8</sup> C. Lacroix, *Solid State Commun.* **54**, 991 (1985).
- <sup>9</sup> F. C. Zhang and T. M. Rice, *Phys. Rev. B* **37**, 3759 (1988).
- <sup>10</sup> R. M. Fye and D. J. Scalapino, *Phys. Rev. B* **44**, 7486 (1991).
- <sup>11</sup> T. Nishino and K. Ueda, *Phys. Rev. B* **47**, 12 451 (1993).
- <sup>12</sup> P. Fazekas and E. Muller-Hartmann, *Z. Phys. B* **85**, 285 (1991).
- <sup>13</sup> N. E. Bickers, *Rev. Mod. Phys.* **59**, 845 (1987).
- <sup>14</sup> A. M. Tsvelik, *Phys. Rev. Lett.* **69**, 2142 (1992).
- <sup>15</sup> P. Coleman, E. Miranda, and A. Tsvelik, *Phys. Rev. Lett.* **70**, 2960 (1993).
- <sup>16</sup> F. A. Berezin and M. S. Marinov, *Pis'ma Zh. Eksp. Teor. Fiz.* **21**, 678 (1975) [*JETP Lett.* **21**, 320 (1975)].
- <sup>17</sup> H. Razafimandimby, P. Fulde, and J. Keller, *Z. Phys. B* **54**, 111 (1984).
- <sup>18</sup> C. M. Varma, *Phys. Rev. Lett.* **55**, 2723 (1985).
- <sup>19</sup> G. M. Éliashberg, *Pis'ma Zh. Eksp. Teor. Fiz.* **45**, 28 (1987) [*JETP Lett.* **45**, 35 (1987)].
- <sup>20</sup> P. Nozieres, *J. Low Temp. Phys.* **17**, 31 (1974).
- <sup>21</sup> A. Yoshimory and H. Kasai, *J. Magn. Magn. Mater.* **31–34**, 475 (1983).
- <sup>22</sup> D. K. Cox, *Phys. Rev. B* **35**, 4561 (1987).
- <sup>23</sup> F. J. Ohkawa, *Phys. Rev. B* **44**, 6812 (1991).
- <sup>24</sup> A. Sumiyama, Y. Oda, H. Nagano *et al.*, *J. Phys. Soc. Jpn.* **55**, 1294 (1986).
- <sup>25</sup> Y. Kitaoka, K. Fujiwara, Y. Kohori *et al.*, *J. Phys. Soc. Jpn.* **54**, 3686 (1985).
- <sup>26</sup> Y. Kitaoka, K. Ueda, K. Fujiwara *et al.*, *J. Phys. Soc. Jpn.* **55**, 723 (1986).
- <sup>27</sup> J. Rossat-Mignod, L. P. Regnault, J. L. Jacoud *et al.*, *J. Magn. Magn. Mater.* **76–77**, 376 (1988).
- <sup>28</sup> D. C. Mattis, *The Theory of Magnetism*, Harper & Row, New York (1965).
- <sup>29</sup> P. Schlottmann, *Phys. Rev. B* **25**, 4828 (1982).
- <sup>30</sup> T. K. Lee, *J. Phys. C* **18**, L31 (1985).
- <sup>31</sup> F. Gandra, S. Schultz, S. B. Oseroff *et al.*, *Phys. Rev. Lett.* **55**, 2719 (1985).
- <sup>32</sup> Yu. Kagan, K. A. Kikoin, and N. V. Prokof'ev, *Pis'ma Zh. Eksp. Teor. Fiz.* **56**, 221 (1992) [*JETP Lett.* **56**, 219 (1992)].
- <sup>33</sup> P. Coleman and N. Andrei, *J. Phys.: Condens. Matter* **1**, 4057 (1989).
- <sup>34</sup> T. Moriya, *Spin Fluctuations in Itinerant Electron Magnetism*, Springer, Berlin (1985).
- <sup>35</sup> Y. Kuramoto, *Solid State Commun.* **63**, 467 (1987).
- <sup>36</sup> T. Moriya, Y. Takahashi, and K. Ueda, *J. Phys. Soc. Jpn.* **59**, 2905 (1990).
- <sup>37</sup> P. Monthoux, A. V. Balatsky, and D. Pines, *Phys. Rev. Lett.* **67**, 3448 (1991).
- <sup>38</sup> C. D. Bredl, S. Horn, F. Steglich *et al.*, *Phys. Rev. Lett.* **52**, 1982 (1984).
- <sup>39</sup> S. Doniach, *Physica B* **91**, 231 (1977).
- <sup>40</sup> C. D. Bredl, F. Steglich, and K. D. Schotte, *Z. Phys. B* **29**, 327 (1977).
- <sup>41</sup> K. Asayama, Y. Kitaoka, and Y. Kohori, *J. Magn. Magn. Mater.* **76–77**, 449 (1988).
- <sup>42</sup> P. Nozieres, *Ann. Phys. (Paris)* **10**, 19 (1985).

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