Journal of Physics: Conference Series **592** (2015) 012090 doi:10.1088/1742-6596/592/1/012090

Renormalization group theory for Kondo breakdown in Kondo lattice systems

K Ballmann, A Nejati and J Kroha

Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Nussallee, 12, 53115 Bonn, Germany

E-mail: kroha@physik.uni-bonn.de

Abstract. We present a renormalization group (RG) theory for the breakdown of Kondo screening in the Kondo lattice model (KLM) without pre-assumptions about the competition between Kondo effect and magnetic ordering or Fermi surface criticality. We show that the vertex between a single, local Kondo spin and the extended conduction electrons obtains RKKY-induced, non-local contributions in the in-and out-going coordinates of scattering electrons due to scattering at surrounding Kondo sites, but it remains local in the Kondo spin position. This enables the existence of a local Kondo screening scale $T_K(y)$ in the KLM, controlled by the effective RKKY coupling parameter y. $T_K(y)$ is determined by the RG flow of the local spin exchange coupling in the presence of the self-consistent spin response on surrounding Kondo sites. We show that $T_K(y)$ exhibits universal behavior and is suppressed by the antiferromagnetic RKKY coupling. Beyond a maximal RKKY parameter value y_{max} Kondo screening ceases to exist even without magnetic ordering. The theory opens up the possibility of describing quantum critical scenarios involving spin wave instabilities or local Kondo breakdown on the same footing.

1. Introduction

One of the intriguing problems of magnetic quantum phase transitions (QPT) in heayy-fermion systems [1] are the conditions for the breakdown of Kondo screening and the destruction of the heavy fermionic quasiparticles. The breakdown mechanisms invoked by different theoretical approaches include critical fluctuations of the local magnetization (local quantum criticality) [2, 3] as well as large Fermi surface fluctuations associated self-consistently with the Fermi volume collapse near the Kondo breakdown [4]. Most recently, Wölfle and co-workers have put forward a scenario of critical quasiparticles, characterized by a diverging effective mass and a slow, non-Fermi liquid powerlaw divergence of the relaxation rate [5, 6]. This scenario of a critical Fermi liquid, based on a self-consistently determinded, singular quasiparticle interaction, is intriguing in its generality, similar in spirit to the Landau Fermi liquid theory, but it does not address which microscopic effect might cause the criticality of quasiparticles. A consistent, microscopic understanding of Kondo breakdown has not been reached. Even without critical fluctuations the local spin-screening scale T_K in Kondo lattice systems is poorly understood.

We have developed a renormalization group theory for local spin screening in dense Kondo systems with RKKY-induced coupling to the surrounding Kondo ions, but in the absence of critical fluctuations. Such a scenario can be realized for temperatures well above the magnetic ordering and above the lattice coherence temperature [7], in two-impurity [8] or in magnetically frustrated lattice systems. We calculate the β-function for the magnetic coupling J between a

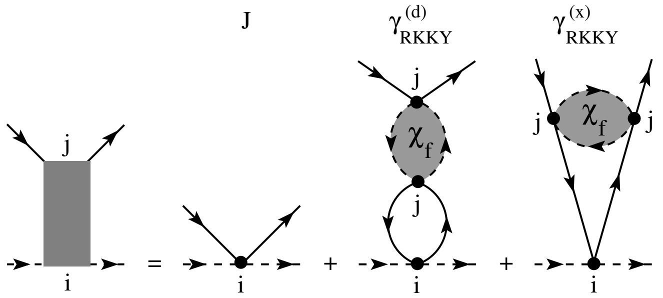

Figure 1. $f-$spin–conduction electron vertex $\hat{\Gamma}$, including all non-local, RKKY-induced contributions to leading order in the spin exchange coupling J_0. Grey bubbles represent the full, $f-$spin susceptibility at sites j. Solid lines depict conduction electrons, dashed lines local f-spins.

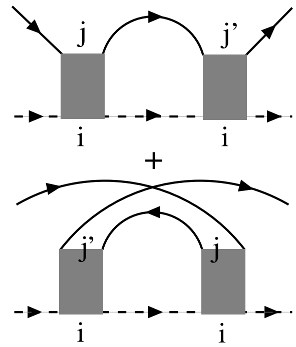

Figure 2. 1-loop diagrams for the perturbative RG. The grey rectangles represent the vertex $\hat{\Gamma}$ of Fig. 1.

localized spin and conduction electrons in 1-loop order, taking into account systematically that in a multi-impurity system the conduction electron – impurity spin vertex has a contribution from the RKKY coupling [9–11] to the surrounding Kondo spins. Since this contribution involves the local dynamical susceptibility on neighbouring Kondo sites, which is inversely proportional [12] to the Kondo spin-screening energy T_K on the neighboring sites, it leads to a self-consistent suppression of T_K. We find that this renormalization of the Kondo scale with respect to the bare Kondo temperature without RKKY coupling, $T_K(y)/T_K(0)$, is a universal function of the dimensionless RKKY coupling parameter y. Remarkably, complete Kondo screening terminates at a maximal RKKY coupling y_{max}, which depends on $T_K(0)$ only. The results are quantitatively consistent with experimental results for tunable two-impurity Kondo systems [8]. This theory reveals that Kondo breakdown may occur even without quantum critical fluctuations. Therefore, it sets the stage for considering Kondo lattice systems with an additional magnetic ordering instability by including critical ordering fluctuations of the incompletely screened magnetic moments in the calculation of the conduction electron-local spin vertex.

The paper is organized as follows. In Section 2 we define the Kondo lattice model and calculate the conduction electron – impurity spin scattering vertex, including systematically the RKKY contributions in leading order of the RKKY coupling y. The one-loop renormalization group equation for this vertex is derived in Section 3, and the universal solutions for the Kondo scale $T_K(y)/T_K(0)$ and the threshold RKKY coupling for Kondo breakdown, y_{max} are presented. We conclude in Section 4 with a discussion of our findings and the implications for future research on quantum criticality in heavy-fermion systems.

2. Kondo lattice model and conduction electron-local spin vertex

The Kondo lattice model (KLM) of localized spins $\mathbf{S}(\mathbf{x}_i)$ on the lattice positions $\mathbf{x}_i$, exchange-coupled to a sea of conduction electrons with dispersion $\varepsilon_{\mathbf{k}}$, is defined as,

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J_0 \sum_i \mathbf{S}(\mathbf{x}_i)\cdot \mathbf{s}(\mathbf{x}_i) \qquad J_0 > 0 \tag{1}$$

where $\mathbf{s}(\mathbf{x}_i) = c^{\dagger}_{i\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}c_{i\sigma'}$ and $\mathbf{S}(\mathbf{x}_i) = 1/2\ f^{\dagger}_{i\tau}\boldsymbol{\sigma}_{\tau\tau'}c_{i\tau'}$ are the spin operators of conduction electrons and of the local spins at site i, respectively. $c_{i\sigma}$, $c^{\dagger}_{i\sigma'}$ denote the local conduction electron operators, $f_{i\sigma}$, $f^{\dagger}_{i\sigma'}$ the fermionic operators of the pseudofermion representation of the local spins with the operator constraint $\hat{Q} = \sum_\sigma f^\dagger_{i\sigma} f_{i\sigma'} = 1$. $\boldsymbol{\sigma}$ is the vector of Pauli matrices, and the sum convention of summing over repeatedly appearing spin indices is adopted. In heavy-fermion systems, the local spins are typically realized by electrons in atomic $4f$-orbitals and will therefore be termed $f-$spins. As is well known, through the antiferromagnetic exchange coupling $J_0 > 0$ this model encompasses both, the formation of local singlets of $f-$spins and conduction spins via the Kondo effect as well as long-range magnetic ordering. The latter is induced by the RKKY interaction which is mediated in $O(J_0^2)$ by the conduction electron density correlations.

As discussed in the introduction, we here investigate the conditions for the Kondo effect, i.e., complete spin screening of a local $f-$spin, to be realized in the Kondo lattice model. In particular, we calculate the temperature scale below which the Kondo singlet is formed. In the language of the perturbative renormalization group (RG) this is the question under which conditions the *full* spin-scattering vertex $\hat{\Gamma}_{fc}$ between conduction electrons and an $f-$spin at an arbitrarily chosen, but fixed site i diverges during the RG flow. Even though the bare spin coupling of the KLM is local, the full vertex $\hat{\Gamma}_{fc}$ acquires non-local contributions, since conduction electrons can scatter from surrounding $f-$spins at sites $j \neq i$ and the flip of an $f-$spin on site j is transfered to the $f-$spin on site i via the RKKY correlations. The corresponding diagrams are shown, to leading (linear) order in the RKKY coupling, in Fig. 1. The first diagram on the right-hand side of Fig. 1 is the bare vertex of the KLM, the second one represents the direct, non-local spin-exchange term, $\gamma^{(d)}_{RKKY}$, and the third one its exchange diagram, $\gamma^{(x)}_{RKKY}$. In this way, the full vertex can be written as,

$$\hat{\Gamma}_{fc}(\mathbf{x}_i, \mathbf{x}_j, i\Omega) = \left[J\delta_{ij} + \gamma^{(d)}_{RKKY}(\mathbf{r}_{ji}, i\Omega) + \gamma^{(x)}_{RKKY}(\mathbf{r}_{ji}, i\Omega) \right] \mathbf{S}(\mathbf{x}_i) \cdot \mathbf{s}(\mathbf{x}_j) \;, \tag{2}$$

with $\mathbf{r}_{ji} = \mathbf{x}_j - \mathbf{x}_i$ the distance vector between the sites i and j and Ω the energy transfered in the scattering process. The solid lines running between the sites i and j depict the RKKY mediated correlations, described by the conduction electron density correlation function $\chi_c(\mathbf{r}_{ji}, i\Omega)$ (bubble of solid lines) in $\gamma^{(d)}_{RKKY}$. In addition, the coupling of the scattering electrons is proportional to the exact, dynamical $f-$spin susceptibility $\chi_f(i\Omega)$ on the surrounding sites $j \neq i$, as also seen in Fig. 1. A detailed calculation shows [13] that the RG flow of $\hat{\Gamma}_{fc}$ is dominated by $\gamma^{(d)}_{RKKY}$ and the exchange part $\gamma^{(x)}_{RKKY}$ gives only a subleading, logarithmic contribution which, in particular, does not influence the universal behavior derived in Section 4. Hence, the $f-c$ vertex reads, to linear order in the RKKY coupling,

$$\hat{\Gamma}_{fc}(\mathbf{r}_{ji}, i\Omega) = J \left[\delta_{i,j} + J_0^2 \; (1 - \delta_{ij}) \; \chi_c(\mathbf{r}_{ji}, i\Omega) \, \tilde{\chi}_f(i\Omega) \right] \mathbf{S}(\mathbf{x}_i) \cdot \mathbf{s}(\mathbf{x}_j) \tag{3}$$

Note that higher order terms, as for instance generated by the RG (see Fig. 2), lead to non-locality of the in-coming and out-going coordinates of the scattering electrons, $\mathbf{x}_j$, $\mathbf{x}_{j'}$, but the $f-$spin coordinate $\mathbf{x}_i$ remains local, because the $f-$spin propagator is strictly local. Therefore, the formation of a lattice-coherent, heavy $f-$band is not relevant for the f-c vertex. The calculation of the dynamical $f-$spin susceptibility for the KLM is, in general, difficult. It are the correlations between spin fluctuations on different lattice sites that have hampered previous treatments of the Kondo lattice problem. However, $\hat{\Gamma}_{fc}$ involves the *local* $f-$spin susceptibility only, whose exact dependence on temperature T is known from the Bethe ansatz solution [12]. It is parameterized by a single energy scale, the single-impurity Kondo temperature T_K and characterized by a $T = 0$ value $\chi_f(0) \propto 1/T_K$ and a crossover to a $1/T$ decay for $T > T_K$. For our analytic treatment, the retarded/advanced dynamical $f-$spin susceptibility can, therefore, be written as,

$$\chi_f(\Omega \pm i0) = \frac{(g_L\mu_B)^2 W}{\pi T_K} \frac{1}{\sqrt{1 + (\Omega/T_K)^2}} \left(1 \pm \frac{2i}{\pi} \mathrm{arsinh} \frac{\Omega}{T_K} \right) =: (g_L\mu_B)^2 \, \tilde{\chi}_f(\Omega \pm i0) \tag{4}$$

where the real part incorporates the exact Bethe ansatz features described above and the imaginary part is implied by the Kramers-Kroenig relation. g_L, μ_B, W are the Landé factor, the Bohr magneton and the Wilson ratio, respectively. The Kondo scale T_K is to be determined self-consistently from the RG solution below.

3. Renormalization group theory for the full $f-c$ vertex

We now construct the one-loop RG equation for the $f-c$ vertex $\hat{\Gamma}_{fc}$, including RKKY-induced non-local contributions to linear order in χ_c. That is, we derive the β−function for the effective coupling constant J of an f−spin at site i to conduction electrons scattering at the Fermi surface, $\mathbf{k}=\mathbf{k}_F$, $\omega=0$. Note that the renormalization of the spin exchange coupling at surrounding sites $j\neq i$ is already incorporated exactly in the full local susceptibility $\chi_f(\Omega\pm i0)$, Eq. (4). Therefore, the bare coupling constant J_0 appears on these sites, as already shown in Eq. (3). The one-loop diagrams are shown in Fig. 2. Note that the dynamical vertex $\hat{\Gamma}_{fc}$ is in general complex (c.f. Eqs. (3), (4)), corresponding to an energy dependent scattering phase. However, for each term of $\hat{\Gamma}_{fc}$ there is its hermitian conjugate term which makes the total scattering vertex in the renormalized Hamiltonian hermitean. Therefore, in leading order of the conduction electron density correlator χ_c, the position dependent part of the one-loop diagrams reads,

$$Y(\mathbf{r}_{ji},\mathbf{r}_{j'i},i\omega,i\Omega)=2\,\mathrm{Re}\left[J^2J_0^2\,\delta_{ij'}\,(1-\delta_{ij})\,G_c(\mathbf{r}_{jj'},i\omega+i\Omega)\,\chi_c(\mathbf{r}_{ji},i\Omega)\,\tilde{\chi}_f(i\Omega)\right]\ , \tag{5}$$

where ω is the energy of in-coming conduction electrons, and $G_c(\mathbf{r}_{jj'},i\omega+i\Omega)$ is the single-particle conduction electron propagator from the in-coming to the out-going sites j and j',

$$G_c(\mathbf{r},\omega\pm i0)=-\pi N(\omega)\,\frac{\mathrm{e}^{\pm ik(\varepsilon_F+\omega)r}}{k(\varepsilon_F+\omega)r}\ , \tag{6}$$

where $r=|\mathbf{r}_{jj'}|$, the bare density of states $N(\omega)$, and $k(\varepsilon_F+\omega)$ is the modulus of the momentum corresponing to the energy ω. Choosing the f−spin site arbitrarily as $\mathbf{x}_i=0$, Fourier transforming the expression Eq. (5) to momentum space and introducing the dimensionless couplings $g=N(0)J$, $g_0=N(0)J_0$, one obtains for in-coming electrons at the Fermi surface,

$$Y(\mathbf{k}_F,\omega=0,i\Omega)=2\,\mathrm{Re}\left[g^2g_0^2\sum_{j\neq 0}\mathrm{e}^{-i\mathbf{k}_F\mathbf{r}_{ji}}\frac{1}{N(0)^4}G_c(\mathbf{r}_{ji},i\Omega)\,\chi_c(\mathbf{r}_{ji},\Omega=0)\,\tilde{\chi}_f(i\Omega)\right]\ . \tag{7}$$

Since χ_c is weakly frequency-dependent on the scale of T_K, it has been replaced by its static, i.e., real part ($\Omega=0$). Integrating in the diagrams of Fig. 2 over the intermediate conduction electron energy and differentiating w.r.t. the running band cutoff D, the RG equation for the local spin-exchange coupling g is obtained in the usual way. Note that the band cutoff appears in both, the intermediate electron propagator G_c and in χ_c. However, differentiation of the latter does not contribute to the logarithmic RG flow, since the RKKY coupling is marginally irrelevant in the RG sense. Nevertheless, χ_c appears as a factor in the RKKY-corrected, local coupling. The 1-loop RG equation ultimately reads,

$$\frac{\mathrm{d}g}{\mathrm{d}\ln D}=-2g^2\left(1-y\,g_0^2\,\frac{D_0}{T_K}\,\frac{1}{\sqrt{1+(D/T_K)^2}}\right)\ , \tag{8}$$

where D_0 is the bare band cutoff and the dimensionless coefficient y is defined via Eq. (7) as

$$y=-\frac{4W}{\pi^2}\sum_{j\neq 0}\mathrm{e}^{-i\mathbf{k}_F\mathbf{r}_{ji}}\frac{1}{N(0)^2}\mathrm{Im}G_c^A(\mathbf{r}_{ji},\Omega=0)\,\chi_c(\mathbf{r}_{ji},\Omega=0) \tag{9}$$

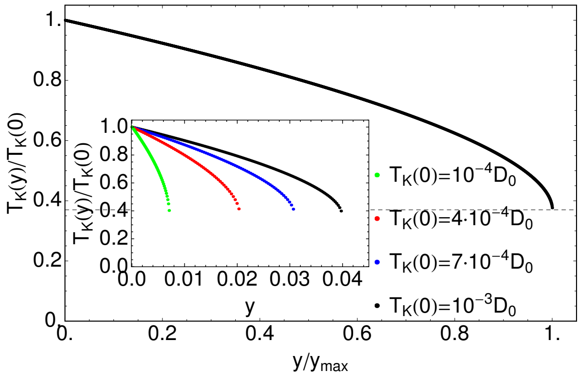

Figure 3. $T_K(y)/T_K(0)$ versus the RKKY parameter y, normalized by y_{max}. The inset shows $T_K(y)/T_K(0)$ for several values of the bare $T_K(0)$.

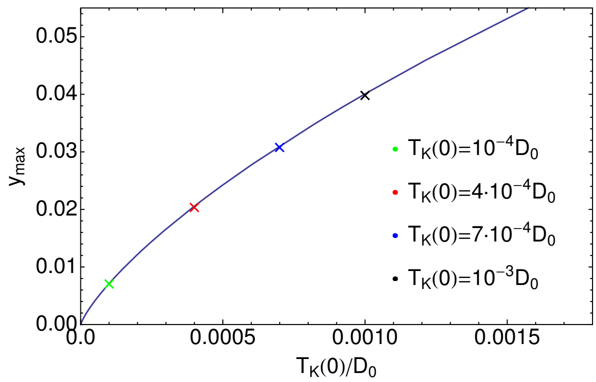

Figure 4. Dependence of y_{max} on $\tau_K = T_K(0)/D_0$, Eq. (12). The crosses indicate the y_{max} values for the $T_K(0)$ values extracted from the inset of Fig. 3.

y parameterizes the RKKY coupling strength. It can be antiferromagnetic ($y > 0$) or ferromagnetic ($y < 0$) due to the spatially oscillating behavior of χ_c. For an isotropic and dense system, $k_F a \ll 1$, the summation in Eq. (9) can be approximated by an integral, and with the substitution $x = 2k_F r$, $r = |\mathbf{r}_{ji}|$, y can be expressed as

$$y \approx -\frac{W}{(k_F a)^3} \int_{k_F a}^{\infty} dx\ (1 - \cos x)\ \frac{x \cos x - \sin x}{x^4} > 0\ , \tag{10}$$

showing generically antiferromagnetic behavior, i.e. a reduction of the effective $f - c$ coupling by the RKKY contributions.

It is seen that the dynamic $f-$spin response χ_f introduces a soft cutoff on the scale of T_K to the RG flow of the RKKY contribution in Eq. (8). More importantly, however, at low energies it is inversely proportional to the local Kondo screening scale T_K. This leads to a negative feedback in the RG flow, which determines the T_K in a selfconsistent way.

4. Universal suppression of the local Kondo scale

The RG Eq. (8) can be integrated analytically. In the perturbative RG framework, T_K is defined as the value of the running cutoff D, where the coupling g diverges. It is then obvious that for the KLM the local Kondo scale depends on the RKKY-mediated coupling y: $T_K = T_K(y)$. The solution of the RG Eq. (8) implies that $T_K(y)$ is self-consistently determined by the equation,

$$\frac{T_K(y)}{T_K(0)} = \exp\left(-y\,\alpha\, g_0^2\, \frac{D_0}{T_K(y)}\right)\ , \tag{11}$$

where $T_K(0) = D_0 \exp(-1/2g_0)$ is the bare Kondo scale without RKKy coupling, and $\alpha = 2\ln(1+\sqrt{2})$. It is readily shown that for sufficiently small y this equation has two solutions, where the larger one (first divergence of g during the RG flow) corresponds to the physical $T_K(y)$. Beyond a maximal antiferromagnetic RKKY strength, $y > y_{max}$, however, Eq. (11) has no solution, i.e. the divergence of the RG and, hence, complete spin screening at the lowest energies ceases to exist. This marks the breakdown of the heavy Kondo quasiparticles. The solutions of Eq. (11) are shown in the inset of Fig. 3 for several bare Kondo temperatures $T_K(0)$. The maximal, RKKY-induced $T_K(y)$ suppression as well as the value of the maximal coupling parameter y_{max} at the Kondo breakdown point can be shown analytically from Eq. (11) to have the universal values [13],

$$\frac{T_{K\,min}}{T_K(0)} = \frac{T_K(y_{max})}{T_K(0)} = \frac{1}{\mathrm{e}}\ , \qquad y_{max} = \frac{4}{\alpha\,\mathrm{e}}\ \tau_K\ (\ln\tau_K)^2\ , \tag{12}$$

where we have defined $\tau_K = T_K(0)/D_0$. Using the definition of $T_K(0)$ above and inserting Eq. (12) into Eq. (11) proves that $T_K(y)$ is suppressed in a universal way, i.e., Eq. (11) is a parameter-free equation for $T_K(y)/T_K(0)$ in terms of y/y_{max} only. Fig. 3 shows the scaling collapse of all $T_K(y)$ curves in terms of the rescaled variables $T_K(y)/T_K(0)$ and y/y_{max}.

5. Conclusion

To conclude, we have shown that in multiple-impurity or Kondo lattice systems the conduction electron-local $f-$spin vertex Γ_{fc} acquires non-local, RKKY-induced contributions from electron spin scattering at surrounding spin sites, but remains local in the $f-$spin coordinate. The perturbative RG treatment of this vertex, including the self-consistently determined response of the surrounding Kondo spins, predicts a universal suppression of the local Kondo screening scale $T_K(y)$ and a breakdown of complete Kondo screening at a finite, maximum RKKY coupling parameter y_{max}. We emphasize that subleading contributions to Γ_{fc}, may modify the form of the cutoff function in the RG Eq. (8) and, therefore, the non-universal parameter α, but they do not change the generic, inverse dependence of the RKKY-induced contributions on the self-consistently determined screening scale. Therefore, subleading contributions do not affect the universal $T_K(y)$ behavior. The universal maximum T_K suppression at the breakdown point, $T_K(y_{max})/T_K(0)$, is in quantitative agreement with the minimal resonance width found in STM spectroscopy on a tunable two-impurity Kondo system [8]. Since the present theory predicts Kondo breakdown without invoking magnetic ordering, it sets the stage for a microscopic description of different quantum critical scenarios on the same footing, driven either by a spin-wave instability of the heavy Fermi liquid when $y < y_{max}$ (Hertz-Millis scenario [14, 15]), or by magnetic ordering of the residual local moments with heavy quasiparticle breakdown when $y = y_{max}$.

References

[1] Von Löhneysen H, Rosch A, Vojta M and Wölfle P 2007 *Rev. Mod. Phys.* **79**, 1015
[2] Si Q, Rabello S, Ingersent K and Smith J L 2001 *Nature* **413**, 804
[3] Coleman P, Pépin C, Si Q and Ramazashvili R 2001 *J. Phys. Cond. Mat.* **13**, R723
[4] Senthil T, Vojta M and Sachdev S 2004 *Phys. Rev. B* **69**, 035111
[5] Wölfle P and Abrahams E 2011 *Phys. Rev. B* **84**, 041101(R)
[6] Abrahams E, Wölfle P and Schmalian J 2014 *Phys. Rev. B* **90**, 045105
[7] Klein M, Nuber A, Reinert F, Kroha J, Stockert O and von Löhneysen H 2008 *Phys. Rev. Lett.* **101**, 266404
[8] Bork J, Zhang Y-H, Diekhöner L, Borda L, Simon P, Kroha J, Wahl P and Kern K 2011 *Nature Physics* **7**, 901
[9] Ruderman M A and Kittel C 1954 *Phys. Rev.* **96**, 99
[10] Kasuya T 1956 *Prog. Theor. Phys.* **16**, 45
[11] Yosida K 1957 *Phys. Rev.* **106**, 893
[12] Andrei N, Furuya K and Lowenstein J H 1983 *Rev. Mod. Phys.* **55**, 331
[13] Ballmann K, Nejati A and Kroha J (to be published)
[14] Hertz J A 1976 *Phys. Rev. B* **14**, 1165
[15] Millis A 1993 *Phys. Rev. B* **48**, 7183