Interorbital pairing for heavy fermions and universal scaling of their basic characteristics

J. Karbowski and J. Spałek*
Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, 00-681 Warszawa, Poland
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We show that the properties of the heavy-electron superconducting state induced by the interorbital kinetic exchange scale with the effective-mass renormalization $m^*/m_0 \sim 1/T_K$. Explicitly, the pairing potential $\tilde{J} \sim J(m_0/m^*)\ln^2(m_0/m^*)$, where J is the magnitude of the bare Kondo coupling; the coherence length $\xi \sim T_K/T_c$, where T_c is the transition temperature, whereas the penetration depth $\lambda \sim (m^*/m_0)^{1/2}$ so that $\lambda/\xi \gg 1$. We also determine the scaling of magnetic critical fields.

In this paper we predict a scaling of fundamental parameters characterizing a heavy-fermion superconductor, which extends the earlier analysis for the normal state.[1] This goal is achieved by considering the Anderson lattice model in which first order corrections in $1/U$, where U is the magnitude of the intra-atomic f-f interaction, have been included[2] so as to generate an interorbital (hybrid) pairing. In this manner, both the Fermi-liquid state of almost localized electrons, as well as their superconducting properties are obtained within a single framework. An earlier treatment[3] of superconductivity within the Anderson lattice model in the $U=\infty$ limit required higher-order $(1/N^2)$ correction to the mean-field slave-boson picture of the heavy electrons. Here, a stable superconducting phase appears already in the mean-field approximation for the pairing part and provides a universal scaling with the mass renormalization m^*/m_0, as discussed below.

We start from the effective Hamiltonian derived earlier[2] to the first nontrivial order in V/U, which was rederived in the slave-boson representation of Zou and Anderson[4] and takes the form

$$\tilde{\mathcal{H}} = \sum_{mn\sigma} t_{mn} c_{n\sigma}^+ c_{n\sigma} + \epsilon_f \sum_{i\sigma} f_{i\sigma}^+ f_{i\sigma} + \sum_{im\sigma} (V_{im} e_i f_{i\sigma}^+ c_{m\sigma} + \text{H.c.}) - \sum_{im} (2V_{im}^* V_{in}/\bar{U}) b_{im}^+ b_{in} , \quad (1)$$

with the pairing operators

$$b_{im}^+ \equiv (f_{i\uparrow}^+ c_{m\downarrow}^+ - f_{i\downarrow}^+ c_{m\uparrow}^+)/\sqrt{2} \quad (2)$$

and $\bar{U} \equiv U + \epsilon_f$.

The first three terms comprise the Anderson lattice model in the $U=\infty$ limit.[1-3] This formulation involves a single scalar boson e_i that has been studied extensively in the last decade,[1] and has been just shown to represent the spinon-holon formulation[4] in the limit $d_i^+ d_i \equiv 0$. The last term expresses the interorbital spin-singlet pairing introduced before,[2,5] here defined for pseudofermions $\{f_{i\sigma}\}$ and conduction electrons $\{c_{i\sigma}\}$. In contradistinction to the one-band (t-J) model situation,[4,6] where the pairing part involves d-d or f-f kinetic exchange, the corresponding term in Eq. (3) expresses for $m=n$, a Kondo-type interaction between the spins.[2] This interaction corresponds to the asymmetric Anderson model with $|V| \lesssim |\epsilon_f - \mu| \ll U + \epsilon_f - \mu$, and hence, is complementary to the symmetric case $|V| \ll |\epsilon_f - \mu| \approx U + \epsilon_f - \mu$ considered by Zhang and Rice.[6] The former situation reflects the heavy-fermion and the fluctuating valence limits. One should stress that the Kondo interaction is regarded here as the source of spin-singlet superconducting pairing in the same way as the kinetic exchange is assumed to provide d-d pairing in a strongly correlated metallic system.[2,6] The problem has been dealt with rigorously for the case of the single pair by Byczuk *et al.*[2] In brief, the Kondo interaction is regarded as the source of binding of pairs into singlets, whereas the residual hybridization [third term in Eq. (1)] introduces the itineracy required for a coherent motion of the singlet pairs.

We now discuss the physical implications of including the last term in Eq. (1) and compare the present results with those obtained earlier in the $U=\infty$ limit[1,2] and with the hybridization of intra-atomic character, specified by $V_{in} = V\delta_{in}$. The partition function Z in the slave-boson representation can be written in a standard way[1,2] as a functional integral over coherent Fermi $\{c_{i\sigma}^+, c_{i\sigma}, f_{i\sigma}^+, f_{i\sigma}\}$ and Bose $\{e_i, e_i^+\}$ fields:

$$Z = \int Dc_\pm Df_\pm De \prod_i d\lambda_i \exp\left[-\int_0^\beta d\tau \left[\sum_i e_i^+ \partial_\tau e_i + \sum_{i\sigma} (c_{i\sigma}^+ \partial_\tau c_{i\sigma} + f_{i\sigma}^+ \partial_\tau f_{i\sigma}) + \tilde{H}_{\text{SB}} \right] \right] , \quad (3)$$

where $\beta \equiv (k_B T)^{-1}$ is the inverse temperature in units of energy, and

$$\tilde{\mathcal{H}}_{\text{SB}} \equiv \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma} + (\epsilon_f - \mu) \sum_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma}^+ f_{\mathbf{k}\sigma} + V \sum_{i\sigma} (f_{i\sigma}^+ e_i c_{i\sigma} + c_{i\sigma}^+ e_i^+ f_{i\sigma}) - (2V^2/\bar{U}) \sum_i b_{ii}^+ b_{ii} + \sum_i \lambda_i \Big(e_i^+ e_i + \sum_\sigma f_{i\sigma}^+ f_{i\sigma} - 1\Big) . \quad (4)$$

The last term in (4) contains a set of Lagrange multipliers $\{\lambda_i\}$ reflecting the local constraint which is imposed at every f site due to the introduction of an extra Bose field $\{e_i\}$. Subsequently, we represent the Bose operator e_i^+ by its space homogeneous part $e \equiv \langle e_i^+ \rangle$, implying the existence of a stable metallic (Fermi-liquid) state and reflecting the spatially extended nature of single-hole (empty) f states. We can also put $\lambda_i=\lambda$, if the mean fermion number is the same at each site. The above (mean-field) approximation for the slave bosons leads to the effective Hamiltonian of the form

$$\tilde{\mathcal{H}}_{SB}\simeq\sum_{\mathbf{k}\sigma}[(\epsilon_{\mathbf{k}}-\mu)c^{+}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+(\tilde{\epsilon}_f-\mu)f^{+}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma} + Ve(f^{+}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+c^{+}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma})] +\lambda N(e^2-1)-(2V^2/\bar{U})\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}b^{+}_{\mathbf{k},-\mathbf{k}+\mathbf{q}}b_{\mathbf{k}',-\mathbf{k}'+q}\ , \tag{5}$$

where $\tilde{\epsilon}_f\equiv\epsilon_f+\lambda$, and $b^{+}_{\mathbf{k},\mathbf{k}'}=(f^{+}_{\mathbf{k}\uparrow}c^{+}_{\mathbf{k}'\downarrow}-f^{+}_{\mathbf{k}\downarrow}c^{+}_{\mathbf{k}'\uparrow})/\sqrt{2}$. The chemical potential μ, and λ, and e are calculated from the free energy ($F=-k_BT\ln Z$) in the saddle point approximation ($\delta F/\delta e=\delta F/\delta\lambda=0$). In the normal state, i.e., when the pairing part is ignored, we recover the principal results obtained before[1,2] in the Kondo-lattice limit $|\epsilon_f-\mu|/\rho_0V^2\gg1$, where ρ_0 is the density of bare states in the conduction band at the Fermi energy μ. Such a condition is fulfilled, e.g., for one electron per (f-c) pair of orbitals and when the bare f level is positioned energetically below the conduction band.

One can easily diagonalize the single-part of (3) and obtain the usual eigenenergies,

$$E_{\mathbf{k}\alpha}=\tfrac{1}{2}\{\epsilon_{\mathbf{k}}+\tilde{\epsilon}_f-2\mu+\alpha[(\epsilon_{\mathbf{k}}-\tilde{\epsilon}_f)^2+(2Ve)^2]^{1/2}\}\ , \tag{6}$$

where $\alpha=\pm1$. The renormalized f-level position $\tilde{\epsilon}_f$ is very close to the Fermi level, as can be seen from the condition $\delta F/\delta e=0$, which at $T=0$, yields

$$\tilde{\epsilon}_f-\mu\sim(W/2)\exp[-(\mu-\epsilon_f)/V^2\rho_0]\ , \tag{7}$$

where the bare band spans from $-W/2$ to $W/2$ and is assumed as featureless. The above energy difference is defined as k_BT_K, where T_K is customarily called the effective Kondo temperature.[1] Additionally, from the condition $\delta F/\delta\lambda=0$, one determines the value of $e^2\equiv1-n_f=k_BT_K/2V^2\rho_0\ll1$, and the density of quasiparticle states at μ as $\rho(\mu)=1/2k_BT_K$. In effect, the effective mass of quasiparticle near the Fermi surface is given by $m^*\sim1/T_K$; therefore, T_K determines the degree of itineracy of the bare electrons (for $T_K=0$, $m^*=\infty$, and all f sites are singly occupied and the electrons are localized). The overall width of the lower hybridized band ($\alpha=-1$) is $D=2|V|e=(2k_BT_K/\rho_0)^{1/2}\simeq(2k_BT_KW)^{1/2}\gg k_BT_K$.

We now extend the scaling of quantities with T_K to the superconducting phase. For that purpose we consider the case for which the number of particles is $n\le2$ per site so that only the lower hybridized band $E_{\mathbf{k}-}\equiv E_{\mathbf{k}}$ is occupied in the temperature range much smaller than the hybridization gap, $k_BT\ll|V|e$. The effective Hamiltonian (5) transformed to the hybridized basis then has the form

$$\tilde{\mathcal{H}}_{SB}=\sum_{\mathbf{k}\sigma}\Psi^{+}_{\mathbf{k}\sigma}E_{\mathbf{k}}\Psi_{\mathbf{k}\sigma}-\frac{V^2}{\bar{U}}\sum_{\mathbf{k}\mathbf{k}'}\frac{4V^2e^2}{[(\epsilon_{\mathbf{k}}-\epsilon_f)^2+4V^2e^2]^{1/2}[(\epsilon_{\mathbf{k}'}-\epsilon_f)^2+4V^2e^2]^{1/2}}\Psi^{+}_{\mathbf{k}\uparrow}\Psi^{+}_{-\mathbf{k}+q\downarrow}\Psi_{-\mathbf{k}'\downarrow}\Psi_{\mathbf{k}'+\mathbf{q}\uparrow}\ , \tag{8}$$

where $\Psi^{+}_{\mathbf{k}\sigma}$ is the creation operator of a hybridized a-c state. The potential is separable into $\mathbf{k}$- and $\mathbf{k}'$-dependent factors. Thus, the $\mathbf{k}$ dependence of the superconducting gap $\Delta_{\mathbf{k}}$ is determined by the $\mathbf{k}$-dependent factor in the denominator. More generally, $\Delta_{\mathbf{k}}\sim V_{\mathbf{k}}$ has nodes for $\mathbf{k}$ points for which $V_{\mathbf{k}}=0$. In our present model situation with $V_{\mathbf{k}}=V$, the gap is never zero; therefore, we approximate the pairing potential by its average over occupied quasiparticle states. This leads to an effective $\mathbf{k}$-independent potential,

$$\tilde{J}\simeq\frac{V^2}{\bar{U}}\left[\frac{k_BT_K}{Ve}\right]^2\ln^2\left[\frac{k_BT_K}{|V|e}\right] =\frac{V^2\rho_0}{4\bar{U}}k_BT_K\ln^2(k_BT_K\rho_0)\ . \tag{9}$$

In the limit of f-electron localization $\tilde{J}\to0$ (note that the pairing takes place when $e\neq0$, i.e., when the f holes exist and propagate). The disappearance of the pairing in the strict Kondo-lattice limit ($e=0,n_f=1$) implies that our approach, indeed, describes pairing, not the singlet Kondo-type of state. For typical values $|V|=0.5$ eV, $e^2=0.06$, $\mu-\epsilon_f=0.8$ eV, $W=2$ eV, $U=6$ eV, we obtain a mean-field superconducting transition temperature $T_c\sim1$ K, a quasiparticle bandwidth $D\simeq3\times10^{-2}$ eV, and $\tilde{J}=5\times10^{-4}$ eV, so that $\tilde{J}/D\approx10^{-2}$. Thus, the mean-field (BCS) approximation is applicable, since $\tilde{J}$ is only a minute fraction of the quasiparticle energy on the Fermi surface. Furthermore, we take advantage of the fact that $\tilde{J}/D\ll1$ and replace the pairing potential in (8) by the average value $\tilde{J}$ and then transform the resulting term back to real space; such a procedure produces a single band of heavy fermions with local pairing of the form $-\tilde{J}\Psi^{+}_{\uparrow}(\mathbf{r})\Psi^{+}_{\downarrow}(\mathbf{r})\Psi_{\downarrow}(\mathbf{r})\Psi_{\uparrow}(\mathbf{r})$ which reduces (8) to a negative U model.[7] The intrasite pairing is allowed because it involves hybridized quasiparticle states which are a mixture of noninteracting pseudofermions $f^{+}_{i\sigma}$ and carriers $c^{+}_{i\sigma}$ and leads to a real-space version of the BCS theory.

The local nature of pairing in conjunction with the single-band nature of the problem allows us to derive explicitly the Ginzburg-Landau functional within the Lagrangian formalism for the Grassmann variables $\Psi^{+}_{\sigma}(\mathbf{r})$ and $\Psi_{\sigma}(\mathbf{r})$. Namely, the above analysis reduces the Lagrangian for the hybridized states with pairing to a form which in the continuous limit reads

$$\mathcal{L}(\tau)=\int d^3x\left\{\sum_{\sigma}\Psi^{+}_{\sigma}[p_0+E(\mathbf{p})]\Psi_{\sigma} -\tilde{J}\Psi^{+}_{\uparrow}(\mathbf{x}),\Psi^{+}_{\downarrow}(\mathbf{x})\Psi_{\downarrow}(\mathbf{x})\Psi_{\uparrow}(\mathbf{x})\right\}\ , \tag{10}$$

where $\Psi_{\sigma}=\Psi_{\sigma}(\mathbf{x},\tau),p_0\equiv\partial_{\tau}$, and $E(\mathbf{p})$ is the eigenenergy

$E_{\mathbf{k}}$ with $\mathbf{k}$ replaced by $(-i\nabla)$. Expression (10) differs from the corresponding expression in the standard BCS theory by the complicated form of $E(\mathbf{p})$, and contains the bare energy $\epsilon_{\mathbf{p}}$, taken as $(-\hbar^2\nabla^2/2m_0)$. We also introduce the two-component Nambu notation $\Psi^+ \equiv (\Psi_\uparrow^+, \Psi_\downarrow)$ in (10) and apply the Hubbard-Stratonowich transformation to the quartic term. Such a procedure reduces the partition function to the form

$$Z = \int D\Psi D\Psi^+ D\Delta \exp\left\{ -\int_0^\beta d\tau \int d^3x \left[\Psi^+ \begin{bmatrix} p_0 + E(\mathbf{p}) & -\tilde{\Delta} \\ -\tilde{\Delta} & p_0 - E(\mathbf{p}) \end{bmatrix} \Psi - \frac{|\tilde{\Delta}|^2}{\tilde{J}} \right] \right\}, \tag{11}$$

with $\tilde{\Delta} = \tilde{J}\Delta$. Integrating over Grassmann variables and neglecting the part which does not depend explicitly on $\tilde{\Delta}$ we obtain

$$Z = \int D\Delta \exp\left\{ \mathrm{Tr}\ln\left[1 - \begin{bmatrix} \dfrac{1}{p_0 + E(\mathbf{p})} & -\tilde{\Delta} \\ -\tilde{\Delta} & \dfrac{1}{p_0 - E(\mathbf{p})} \end{bmatrix} \right] - \beta \int d^3x |\tilde{\Delta}|^2/\tilde{J} \right\}, \tag{12}$$

where the part $\{\cdots\}$ is called the effective action S_{eff}. Expanding $\exp(-S_{\text{eff}})$ into a Taylor series, carrying out a Fourier expansion, and evaluating corresponding sums,[8] one arrives at the Ginzburg-Landau functional E_{GL} in the form

$$F_{\text{GL}} = -\frac{1}{2}\rho_0 \frac{m^*}{m_0} \int_0^\beta d\tau \int d^3x \left\{ \left[\left[1 - \frac{T}{T_c} \right] + \xi^2 \nabla^2 \right] \times |\tilde{\Delta}|^2 - \frac{7}{16} \frac{\zeta(3)}{\pi^2 T_c^2} |\tilde{\Delta}|^4 \right\}, \tag{13}$$

with $T_c = 1.13 D \exp[-1/\tilde{J}\rho(\mu)] \sim T_K^{1/2} \exp(-k_B T_K/\tilde{J})$. The coherence length at $T=0$ is

$$\xi_0^2 = \frac{7}{48} \frac{\zeta(3)}{\pi^2 T_c^2} \left[\frac{k_B T_K}{D} \right]^4 \frac{k_F^2}{m_0^2} \sim (T_K/T_C)^2 , \tag{14}$$

with k_F being the Fermi wave vector and $\zeta(x)$ the Riemann zeta function.

To determine the London penetration depth we start with the substitution $\nabla \to \nabla - (2ie_0/c)\mathbf{A}$, where $\mathbf{A}$ is the vector potential and e_0 is the electron charge. This produces the term $(1/2)m_A^2 \mathbf{A}^2$ in S_{eff}, where

$$m_A^2 = \frac{2}{3} e_0^2 \left[\frac{v_F}{c^2} \right]^2 \left[1 - \frac{T}{T_c} \right] \left[\frac{k_B T_K}{Ve} \right]^5 \times \rho(\mu) \sim k_B T_K (1 - T/T_c) m_{\text{BCS}}^2 ,$$

is the photon mass in the superconducting phase, and $m_{\text{BCS}}^2 = 2e_0^2(v_F/c)^2\rho_0/3$ is the mass if there were no enhancement due to the presence of the f level. The London penetration depth at $T=0$ is $\lambda_0 = (\hbar/m_A) \sim T_K^{-1/2}$. The last quantity enters the ratio $\kappa = \lambda/\xi$, which takes the form

$$\kappa = [\sqrt{2/3}\,\xi_0 e_0 v_F (\tilde{\epsilon}_f/|V|e)\sqrt{\rho_0}]^{-1} \sim T_K^{-3/2} T_c .$$

Note that we have used the relation $\xi \equiv \xi(T) = \xi_0/(1 - T/T_c)^{1/2}$. Also, we have separated the T_c factor from the mass enhancement to separate the pairing-mechanism-dependent factor from the universal features. Close to the f-electron localization, $T_K \to 0$ and then $\kappa \gg 1$.

Expression (13) can be used to determine the thermodynamic critical magnetic field B_C via the relation $B_c^2/2 = -F_{\text{GL}}/V_0$, where V_0 is the volume of the system. Explicitly,

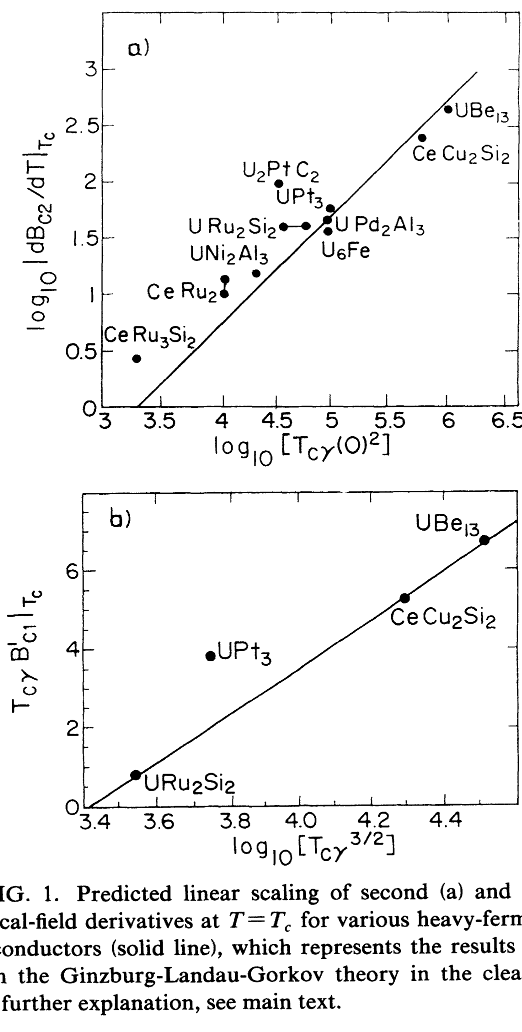

FIG. 1. Predicted linear scaling of second (a) and first (b) critical-field derivatives at $T=T_c$ for various heavy-fermion superconductors (solid line), which represents the results coming from the Ginzburg-Landau-Gorkov theory in the clean limit. For further explanation, see main text.

$$B_C=\left[\frac{2\pi^2}{7\zeta(3)}\rho(\mu)\right]^{1/2}(T_c-T)\sim(T_c-T)T_K^{-1/2}\ , \tag{15}$$

and therefore, the first and second critical magnetic fields are

$$B_{C1}=(\Phi_0/2\pi\lambda^2)\ln(\lambda/\xi)\sim T_K\ln(T_K^{-3/2}T_c a)\ , \tag{16}$$

where a is a constant, and

$$B_{C2}=\sqrt{2}\kappa B_C=2\left[\frac{3\pi^2}{7\zeta(3)}\right]^{1/2}\frac{1}{\xi_0 e v_F}\left[\frac{Ve}{\tilde{\epsilon}_f}\right]^2 \sim(T_C/T_K^2)(T_C-T)\ . \tag{17}$$

The numerical estimates of the quantities calculated above are for the values of parameters specified as follows: $\xi_0\sim10^2$ Å, $\lambda_0=(D/k_BT_K)\lambda_0^{\rm BCS}\gtrsim10_0^{\rm BCS}$, where the label BCS means the value for the BCS theory with the same coupling constant and the same Fermi wave vector k_F, but with no mass enhancement. These results reflect the trends observed experimentally.[9] A detailed comparison requires extraction of the effective masses from the linear specific-heat coefficient $\gamma(0)\sim T_K^{-1}$, as well as the knowledge of other parameters. Specifically, we have calculated the derivative $B'_{c2}=-(dB_{C2}/dT)$ at $T=T_c$ and have plotted it as a function of $T_c\gamma^2$, as displayed for various systems in Fig. 1(a). The systems with large γ scale linearly, as predicted by Eq. (17). Moreover, the slope for the systems UBe_{13}, $CeCu_2Si_2$, and UPt_3 is very close to unity, as predicted by (17). The data were extracted from the works listed in Ref. 10. Only the systems with large mass should scale precisely, as one can see from detailed calculations. In Fig. 1(b), we have plotted the quantity of $B'_{c1}\equiv|dB_{c1}/dt|$ at $T=T_c$ as a function of $\gamma^{3/2}T_c$; the experimental values for various systems are also marked.[11] The solid line represents predicted scaling, which is not fulfilled for UPt_3. Clearly, the clean limit scaling represents the trends of the data.

In summary, we have presented a semiquantitative and universal scaling of both normal and superconducting properties of heavy fermions, taking into account processes of the order V^2/U, which produce the hybrid pairing. We have reduced the problem to the one-band form and on this basis have derived the Ginzburg-Landau functional. Even though $F_{\rm GL}$ is of standard form, the coefficients acquire unusually high values because of the factor m^*/m_0 in Eq. (13). In general, one should also include the scaling with temperature of the effective mass; this follows from the low-temperature expansion, which leads to $\tilde{\epsilon}_f(T)=k_BT_K[1+(T/T_K)^2]$. Similarly, $e^2(T)=e^2[1-(T/T_K)^2]$. These renormalizations will introduce non-BCS corrections to the T dependence of the fundamental parameters, as will be discussed elsewhere. Finally, the effect of f-f exchange interactions, as well as of the hybridization $V_{\rm K}$ anisotropy must be included before a quantitative analysis of superconductivity of heavy fermions, coexisting with itinerant antiferromagnetism in systems like UPt_3, is undertaken.

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*Also at Superconductivity Research Center, 1396 Physics Building, Purdue University, West Lafayette, IN 47907-1396.

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