Comment on "Effective Magnetic Moments of Heavy Fermions and the Wilson Ratio for Kondo Lattices"

Zou and Anderson (ZA)[1] have proposed an explanation for small Wilson ratios (R) obtained[2] for some heavy-fermion superconductors. ZA perform an effective band calculation in which two of six $J=\frac{5}{2}$ states per Ce atom hybridize with a spin-$\frac{1}{2}$ free-electron band, as shown in Fig. 1. Note that T_K and $\tilde{V}(\sim\sqrt{D}T_K)$[3,4] correspond to ZA's ϵ_0 and α, respectively. The renormalized Fermi-level density of states per spin $\tilde{N}(0)$ is given by $\tilde{N}(0)/N(0)=(\tilde{V}/T_K)^2=m^*/m$. ZA have shown that the zero-temperature Pauli susceptibility $\chi_P(0)$ for the lower $(-)$ band is given by

$$\chi_P(0)=\mu_P^2[2\tilde{N}(0)]=1.16\mu_B^2[2\tilde{N}(0)]. \quad (1)$$

I wish to point out that consideration of (i) Van Vleck terms omitted by ZA and (ii) a model including crystalline-electric-field (CEF) splitting shows that the effective moment $\mu_{\rm eff}$ one should use in R appears in the ionic (zero hybridization) Curie law.

With notation as per Fig. 1, the Van Vleck susceptibility $\chi_{VV}(0)$ is

$$\chi_{VV}(0)=\sum_p\langle|\langle\tfrac{5}{2}k\uparrow|\mu_z|\tfrac{5}{2}kp\rangle|^2\rangle_{FS}\mu_B^2[2\tilde{N}(0)] \quad (2)$$

$$=(g_J^2J(J+1)\mu_B^2/3-\mu_P^2)[2\tilde{N}(0)]. \quad (3)$$

Here $\langle\,\rangle_{FS}$ denotes an angular average over the Fermi surface, and $\mu_z=l_z+2S_z$ is the usual magnetic moment operator. $\chi_{VV}(0)\sim\chi_P(0)$ because the Van Vleck energy denominator is precisely $T_K\sim\tilde{N}(0)^{-1}$ (see Fig. 1). Equation (3) follows from inserting a complete set of f states in (2) (including the $J'=\frac{7}{2}$ excited manifold). Here $g_J=\frac{6}{7}$.

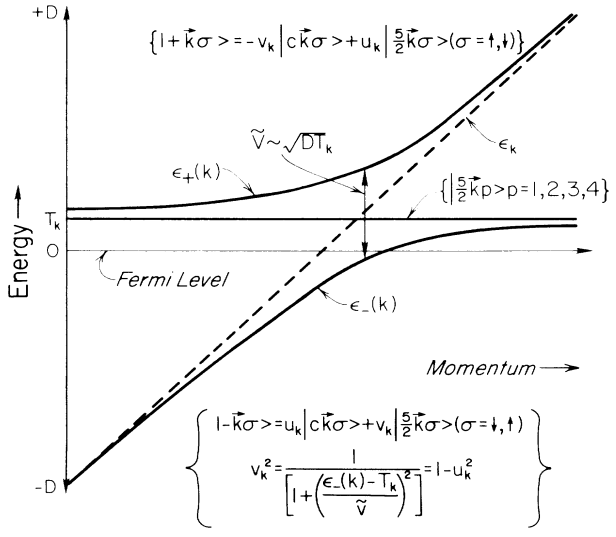

FIG. 1. ZA effective band model. ϵ_k is the bare conduction-band dispersion, and $\{|\frac{5}{2}\mathbf{k}p\rangle\}$ the unhybridized f bands.

TABLE I. Model properties. Note $N=2J+1$.

Model	$\left(\frac{\mu_{\rm eff}}{\mu_B}\right)^2$	$3\chi(0)$	$\frac{3\gamma(0)}{(\pi k_B)^2}$	$3(k_BT)\chi(T)\vert_{T,\tilde{V}=0}$
ZA [a]	$g_J^2(J+1)$	$2\tilde{N}(0)\mu_{\rm eff}^2$	$2\tilde{N}(0)$	$\mu_{\rm eff}^2$
SU(N) [b]	$g_J^2(J+1)$	$N\tilde{N}(0)\mu_{\rm eff}^2$	$N\tilde{N}(0)$	$\mu_{\rm eff}^2$
CEF	$3g_\Gamma^2$	$2\tilde{N}(0)\mu_{\rm eff}^2$	$2\tilde{N}(0)$	$\mu_{\rm eff}^2$

[a]Reference 1. [b]Reference 3.

The net $\chi(0)$ value and linear specific-heat coefficient $\gamma(0)$ are given in Table I. In view of the conventional definition $R=(\pi k_B/\mu_{\rm eff})^2[\chi(0)/\gamma(0)]$,[2,5] it is clear that $\mu_{\rm eff}^2=(2.54)^2\mu_B^2$ for both ZA's model and the less realistic SU($N=6$) effective band model considered elsewhere.[3]

Now consider a model with CEF splitting $\Delta_{CEF}\gg T_K$, with f levels of cubic Γ_7 symmetry having total ionic Zeeman splitting in applied field h of $2g_\Gamma\mu_Bh$. The angular dependence forced by cubic symmetry leads to the combination of squared matrix elements of μ_z appearing in $\chi(0)$ to be g_Γ^2 over the Fermi surface except for a few regions of angular width $\sim(m/m^*)^{1/2}$.

Thus, in all cases (see Table I), the correct $\mu_{\rm eff}$ value is read off from the zero hybridization (free ion) Curie law. For $CePd_3$, $CeSn_3$, and α-Ce ($\Delta_{CEF}\ll T_K$ so $\mu_{\rm eff}=2.54\mu_B$) the R values are 1.4, 0.9, and 1.4, respectively.[5] For $CeCu_2Si_2$, ($\Delta_{CEF}\gg T_K$)$\chi(0)=0.019$ emu/mole (along the c axis),[6] $\gamma(0)=1000$ mJ/mole-K,[2,7] and $\langle\Gamma_7|\mu_z|\Gamma_7\rangle=1.08$,[8] so $R=1.2$.

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