

Anderson and Zou Respond: We welcome the comments of Zhang and Lee, Aeppli, and Varma, and Cox. Their main point is the same and our answer is the same. As far as we can see, their calculation of the “Van Vleck susceptibility” is roughly correct within a straightforward, perhaps somewhat oversimplified interpretation of our model; somewhat oversimplified because we believe that some of the f occupation is caused by hybridization with free-electron states rather far from the Fermi level, while they have assumed an essentially flat band. If one does a band calculation and simply “squashes” the bands by a factor m/m^* their result is roughly correct.

The actual reason why we believe that the Van Vleck terms are small is more subtle. As far as we can see, in the final stage of renormalization caused by the strong frequency dependence of the self-energy, the Van Vleck terms in χ do not share in the renormalization upward but remain the same size as they are in the bare hybridization model, of order μ^2/Δ (Δ is the width of the bare f resonance) rather than $\mu^2/Z\Delta = \mu^2/T_K$, which is the size of the diagonal, Pauli-type term (in a heavy-fermion system, $Z \sim m/m^*$). The missing susceptibility is restored by the effective quasiparticle interaction $I(q)$. The most direct way to see this is to think in terms of first doing band theory for the ground and low excited states, and then turning on the strong interactions which cause the large renormalization of χ of order $Z^{-1} = m^*/m$. There is no reason for the Van Vleck terms to renormalize with this factor. The more physical but less transparent route from disordered moments at high T to singlets at low T makes this process look mysterious when it is not.

The Pauli contribution, rather miraculously, does renormalize along with the effective mass, because the angular momentum \mathbf{J} is conserved in every internal scattering event within the f shell, these scattering events being responsible for the Kondo resonance. Another way to say it is that the diagonal part of the magnetic field perturbation, i.e., that due to the component of H along k , H_k , does not rotate the internal structure of the f -shell atoms relative to k and, equally, does not modify the phase relations between the free-electron part of ψ_k and the internal part. The band wave function has a diagonal element of the perturbation due to the field,

$$\langle k | V_H | k \rangle = g_k \mu H_k,$$

and this is retained in the renormalization of the density of states by Z in the bare-to-quasiparticle transformation.

The off-diagonal matrix element between bands, however, comes from the part of the perturbation which rotates the internal f states into states orthogonal to the original one. This makes them by definition orthogonal to the free-electron part of the quasiparticle wave func-

tion and destroys the coherence properties between internal and external regions. It is not even clear that there are any quasiparticle poles corresponding to the “flat bands” which do not interact with free electrons; and in any case the states reached by the Van Vleck terms are in the high-frequency tails of the appropriate quasiparticle Green’s function if any. Therefore, we believe that the mechanism of Zou and Anderson accounting for the small observed χ is literally correct. In fact, with more complicated band structures it might be that even less of $\mathbf{M} \cdot \mathbf{H}$ remains diagonal in the quasiparticle operators.

The neutron experiments cannot distinguish quasiparticle and off-diagonal contributions to χ , since the neutron interacts with the “bare” particle susceptibilities and hence couples primarily to a many-quasiparticle continuum. The single-quasiparticle pair contribution to $\text{Im}\chi(q, \omega)$ will be extremely small, of order $< m/m^*$. Here we propose a distinct experiment to settle this argument: Since SmB_6 is an insulator¹ at very low temperature, the Pauli susceptibility should vanish when the gap is fully developed. Therefore one can directly measure the Van Vleck susceptibility of a very pure SmB_6 sample at low T , although one has to subtract the “intrinsic Van Vleck contribution” due to the configuration splitting between the $J=0$ and $J=1$ states, which has nothing to do with χ discussed here, from the total χ .

We did not mean to rely too naively on the single-impurity idea, though we admit that our ideas are evolving on this matter. We feel that the effective quasiparticle interaction $I(q)$ (which is equivalent to a “polarization potential”) is indeed q dependent and reflects (probably antiferromagnetic) correlations between neighboring f shells. Nonetheless, we find it hard to believe that its primary effect is not repulsion between antiparallel spins, and hence we believe that it does increase $\chi(q)$ at all q , if more so at large q , according to

$$\chi(q) = \chi_0 / [1 - I(q)\chi_0].$$

Our ideas on those matters were much clarified by discussions with D. Pines, J. Sauls, S. Coppersmith, and C. M. Varma. We thank B. Batlogg for experimental information on SmB_6 .

P. W. Anderson and Z. Zou
Department of Physics
Princeton University
Princeton, New Jersey 08544

Received 31 March 1987
PACS numbers: 75.20.En, 75.20.Hr

¹See, for example, A. Menth, E. Buehler, and T. H. Geballe, Phys. Rev. Lett. **22**, 295 (1969).