# Disorder and coherence in heavy-fermion systems

Zlatko Tešanović
*Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138*
(Received 8 May 1986)

The effects of disorder on the formation of the coherent state in heavy-fermion systems are studied. The renormalized heavy band, characterized by an effective hybridization parameter, is destabilized by a critical strength of impurity scattering leading to self-energy corrections of order $T_K$. For a higher degree of disorder the heavy-fermion system will behave much like a collection of independent Kondo impurities, lacking the characteristic signatures of coherence in resistivity, specific heat, etc. The substitution of impurities on the conduction-electron side has a little influence on coherence; most of the effect comes from the strength of impurity scattering on the $f$-electron sites. The results are discussed in connection with experimental data.

The discovery of superconductivity[1-3] and other anomalous properties of heavy-fermion compounds has led to intense theoretical[4] and experimental[5] activity in an effort to understand the physics of this new class of metals. It has become increasingly clear that there is a need to understand precisely the normal state of these materials, frequently referred to as a Kondo lattice state, before more exotic problems concerning superconductivity can be successfully resolved.

One of the most intriguing characteristics of heavy-fermion materials is the development of "coherence" in their low-temperature properties. In the standard dilute-impurity systems as the temperature decreases below $T_K$ ($T_K$ is the Kondo temperature which determines the energy scale for a single magnetic impurity in metal) the quantities like resistivity and the specific-heat coefficient show a monotonic rise, saturating to a maximum at zero temperature. This behavior is now well understood theoretically both from the numerical calculation using the renormalization group[6] and from the analytical approaches using Bethe ansatz results.[7] In heavy-fermion systems, however, the resisitivity reaches a maximum at some finite temperature $T_0$, which is generally lower than $T_K$ and then decreases sharply to a relatively low value at $T=0$.[5] Similar manifestations of coherence have been observed in other quantities and there seems to be plenty of evidence that at $T \ll T_0$ the behavior of most of the heavy-fermion compounds is consistent with that of the strongly renormalized Fermi liquid, with itinerant heavy electrons having the effective mass of order $10^3$ coherently propagating through a lattice. The question of the formation of this coherent state in the Kondo lattice, and the nature of the residual interactions of the heavy electrons constitute a major challenge in this field.

While at present there is no complete answer to the above questions there is a reasonably uniform picture emerging from various approximate treatments of the periodic Anderson Hamiltonian, which is a usual starting point in studies of the Kondo lattice problem. Despite differences in details, most of these approaches, which in the end employ some form of variational or mean-field approximations,[8] predict that at $T=0$, or at $T \ll T_0$, the heavy-fermion behavior arises through the coherent hybridization of the $c$- and $f$-electron derived bands, resulting in the enhancement of density of states at the Fermi level. This enhancement is described by an effective hybridization parameter strongly renormalized from its bare value due to interactions.

In this paper I study the effects of random disorder on the self-consistent solution to the Anderson lattice Hamiltonian. I will be working within the framework of the $T=0$ Kondo boson field theory (KBFT) (Ref. 9) but qualitatively similar results could be reached using other approaches listed in Ref. 8. In KBFT the intrasite Coulomb repulsion $U$ is set to infinity which restricts the occupancy of the $f$ level to zero or one. This restriction is accomplished by introducing additional Bose fields $b_i$ for each site and writing the Anderson Hamiltonian as

$$H_{\mathrm{KB}} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_i \sum_{m=1}^{N_f} E_f f^{\dagger}_{im} f_{im} + \frac{1}{\sqrt{N_f}} \sum_{i,m,\mathbf{k}} V b_i f^{\dagger}_{im} c_{im\mathbf{k}} + \mathrm{H.c.}\,, \tag{1}$$

where $c_{im\mathbf{k}}$ projects out the $m$th aximuthal angular-momentum state around the site $i$ out of the conduction-band state, $-E_f<0$ is the bare energy of the $f$ level, $V$ is the hybridization matrix element, and $N_f$ is the degeneracy of the $f$ level. With this Hamiltonian the operator $Q_i = b_i^{\dagger} + n_{f_i}$ is conserved. By restricting to the subspace in which $Q_i = 1$ the double occupancy of the $f$ sites is eliminated.

The mean-field approximation for $H_{\mathrm{KB}}$ consists of replacing the operator $b_i$ by a $c$ number. In the "clean" case the lattice periodicity requires that $b_i$ is the same at every site. The theory now has two parameters, $b$ and the Lagrange multiplier $\lambda$ introduced to assure that $Q_i = 1$; the values of these parameters which minimize the total free energy are determined from the set of self-consistent equations,

 

$$\lambda b = -\frac{1}{N_f}\sum_{km} V\langle c^{\dagger}_{imk} f_{im}\rangle \ , \tag{2}$$

$$\langle n_{f_i}\rangle = 1-b^2 \ . \tag{3}$$

The $b\neq 0$ solution to Eqs. (2) and (3) becomes possible for temperatures less than

$$T_{\rm MF} = 1.14D\exp[-E_f/N(0)V^2] \simeq T_K \ ,$$

where $D$ is the width and $N(0)$ is the density of states in the conduction electron band. Below $T_{\rm MF}$ there is a coherent hybridization of the $c$- and $f$-electron states with $bV$ playing the role of the effective hybridization matrix element. The mean-field solution is shown to be exact in the $N_f \to \infty$ limit.[10] For finite $N_f$ the fluctuations are expected to alter the mean-field result; still, as long as $N_f$ is large and $T \ll T_{\rm MF}$ we can assume that the mean-field solution is qualitatively correct. At $T=0$, in particular, it is equivalent to a number of other models.[8]

The disorder is simulated by the extra piece $H_{\rm dis} = \sum_i H_{{\rm dis}_i}$ which we add to the the Anderson Hamiltonian,

$$H_{{\rm dis}_i} = W_{f_i} f_i^{\dagger} f_i + W_{c_i} c_i^{\dagger} + W_{fc_i} b_i f_i^{\dagger} c_i + {\rm H.c.} \tag{4}$$

Potentials $W_{f_i}$, $W_{c_i}$, and $W_{fc_i}$ are taken to be Gaussian random variables satisfying the following relations:

$$\langle W_{f_i}\rangle = \langle W_{c_i}\rangle = \langle W_{fc_i}\rangle = 0 \tag{5}$$

and

$$\langle W_{f(c,fc)_i} W_{f(c,fc)_j}\rangle = W^2_{f(c,fc)}\delta_{ij} \tag{6}$$

where $\langle\ \rangle$ denotes the average over randomness. $H_{\rm dis}$ describes the most general effect of random impurities; in heavy-fermion systems these effects can involve lattice stresses and imperfections, the substitution of La for Ce and Lu for U, the substitution of impurities on the conduction electron side, etc.

In the presence of disorder, lattice periodicity is lost and $\lambda_i$ and $b_i$ will generally vary from site to site. If the disorder is weak, however, i.e., if the self-energy corrections arising from $W$ are small compared to

$$V^2 b^2 (T=0)/D \simeq T_K \ ,$$

we can average over the disorder using a perturbation expansion. This will lead to a theory in which $\lambda_i$ and $c$ number $b_i$ are replaced by their averages; these averages are then self-consistently determined from Eqs. (2) and (3) appropriately modified to reflect the presence of disorder.

This modification involves finding the self-energy corrections arising from the random impurity scattering and inserting the disorder averaged $G_{f_c}(\mathbf{k},\omega)$ in Eq. (2). To find the self-energy we employ the self-consistent Born approximation (SCBA). For simplicity, and to make the notation more compact, we now set $N_f = 2$ and drop the spin indices in the rest of the paper; we also choose to write equations in a more convenient matrix form defined by the following representation for the Green's function in the absence of disorder,

$$G_0(\mathbf{k},\omega) = \begin{vmatrix} G^0_f(\mathbf{k},\omega) & G^0_{fc}(\mathbf{k},\omega) \\ G^0_{cf}(\mathbf{k},\omega) & G^0_c(\mathbf{k},\omega) \end{vmatrix} \ . \tag{7}$$

In the SCBA the self-consistent equation for the self-energy matrix $\Sigma(\omega)$ can be written as follows:

$$\Sigma(\omega) = \sum_{\mathbf{k}} W G(\mathbf{k},\omega) W \ , \tag{8}$$

where

$$G^{-1}(\mathbf{k},\omega) = G_0^{-1}(\mathbf{k},\omega) - \Sigma(\omega) \ ,$$

and form of the matrix $W$ is obvious from Eqs. (4) and (6). Equation (8), together with (2) and (3), now forms a set of coupled equations from which $b$, $\lambda$, and $\Sigma(\omega)$ are to be found.

This set has, in general, quite a complicated structure and one has to look for a numerical solution. Some of the overall qualitative features are, however, evident. Firstly, there is a decrease in the value of the effective hybridization matrix element $bV$ as the disorder is turned on. The presence of impurities and imperfections therefore does affect the formation of the coherent band of heavy quasiparticles. For some critical degree of disorder $bV=0$, and for stronger disorder there will be no self-consistent solution for the renormalized band. If, in order to make the equations more tractable, we set $W_{fc}=0$ and also assume $W_f = W_c = W$, the critical value is

$$W^{\rm crit} = 1.9V^2 b_0^2 (T=0)/D \simeq T_k \ ,$$

where $b_0$ is solution in the absence of disorder. Figure 1 shows $b/b_0$ as a function of $W$. Another parameter of the theory, the "chemical potential" $\lambda$, is only slightly changed in the presence of disorder.

Secondly, there is a large disparity in the effects on coherence arising from disorder on the $f$- and $c$-electron sites. To produce a considerable depression of $b$, $W_f$ has to be of order $T_K$, while $W_c$ has to be of order $D$. Consequently, a significant disorder of the conduction band is

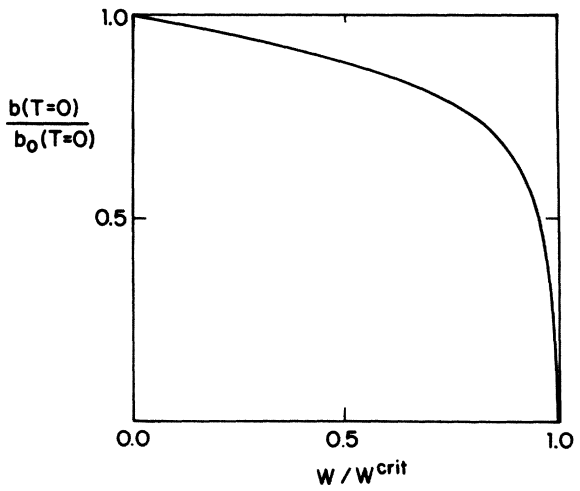


FIG. 1. Effective hybridization matrix element as a function of the degree of disorder.

necessary to affect the coherent band formation. This can be illustrated by evaluating the reduction in $T_{\rm MF}$ produced by disorder. While the mean-field approximation may not be entirely reliable at $T \cong T_{\rm MF}$ the advantage is that the calculations can be performed analytically. The same conclusions can be reached by a numerical calculation of $b(T=0)$. For simplicity we again set $W_{fc}=0$ and proceed by writing down a form of Eq. (2) linearized in $b$,

$$\lambda b = -V^2 \sum_{\mathbf{k},\omega} \frac{b'}{[i\omega + E_f - \lambda - \Sigma_f(i\omega)][i\omega - \xi_{\mathbf{k}} - \Sigma_c(i\omega)]} , \tag{9}$$

where

$$\frac{b}{b'} = 1 + W_c W_f \sum_{\mathbf{k},\omega} \frac{1}{[i\omega + E_f - \lambda - \Sigma_f(i\omega)][i\omega - \xi_{\mathbf{k}} - \Sigma_c(i\omega)]} \tag{10}$$

and $\Sigma_f(i\omega)$ and $\Sigma_c(i\omega)$ are determined self-consistently from Eq. (8). $\sum_\omega$ denotes the sum over the Matsubara frequencies. Assuming that $W_f \ll T_K$ and $W_c \ll D$, Eq. (9) can be rewritten in the following compact form:

$$\ln\left[\frac{T_{\rm MF}}{T^0_{\rm MF}}\right] = -\frac{W_f^2}{2(2\pi)^2 T^{02}_{\rm MF}} + \frac{N(0) W_f W_c}{2T^0_{\rm MF}} - \frac{2N(0)W_c^2}{D} \ln\left[\frac{D}{T^0_{\rm MF}}\right] , \tag{11}$$

where $T^0_{\rm MF}$ is the solution for zero disorder.

From (11) it is clear that if $W_f$ and $W_c$ are of the same order the contribution from the first term dominates, those from the second and third term being a factor of order $(T_K/D)$ and $(T_K^2/D^2)\ln(D/T_K)$ smaller, respectively. The contribution of the last two terms becomes comparable to that of the first term only if $W_c/W_f \simeq D/T_K \sim O(10^3)$. Thus, unless the conduction band is substantially disordered (i.e., $W_c \cong D$), the depression of $T_{\rm MF}$ and, of course $b(T=0)$, are determined by the size of random potential on the $f$ sites. This result is less surprising when one realizes that the spectral weight of the $f$ electrons at the Fermi level is a factor of $\sim D/T_K$ larger than that of $c$ electrons.[11]

Most of the low-temperature properties of heavy-fermion compounds are dominated by the large peak in the electronic density of states arising from heavy band formation. To calculate the density of states for finite disorder it is necessary, for the most general case, to solve three coupled integral equations. This is exceedingly complicated and we again simplify the problem by setting $W_{fc}=0$. The dynamical density of states is defined as

$$N(\omega) = -\frac{1}{\pi} \mathrm{Im} \sum_{\mathbf{k}} \mathrm{Tr} G(\mathbf{k},\omega) , \tag{12}$$

where $G(\mathbf{k},\omega)$ is the full Green's function determined by solution to Eq. (8). The results for $N(\omega)$ are presented in Fig. 2. In real heavy-fermion systems $D/T_K \sim O(10^3)$: As a result it is quite difficult to draw a figure clearly exhibiting all the structure in the density of states. To make the figure legible I have chosen to plot the results for $D/T_K = 10$ which illustrate the same qualitative behavior.

For zero disorder we obtain a familiar structure resulting from the hybridization of the two bands.[8] If the Fermi level is placed in the region of the enhanced density of states right below the gap the low-frequently quasiparticle excitations will be "heavy fermions" with effective mass of order $D^2/b^2V^2 \simeq D/T_K$. As the disorder is turned on, the sharp features are gradually smeared and the peak is significantly reduced. Finally, for $W = W^{\rm crit}$ the initial structure is completely washed out. It is tempting to associate the typical structure in Fig. 2(c) with the shape of density of states inferred from the specific-heat experiments of Bredl *et al.*[12] and, in particular, to identify the halfwidth of a "pseudogap" with the "coherence" temperature $T_0$. However, a word of caution is necessary here since $T_0$ is probably dependent on the residual interactions between heavy fermions, which are ignored in the mean-field approximation. At any rate, it appears

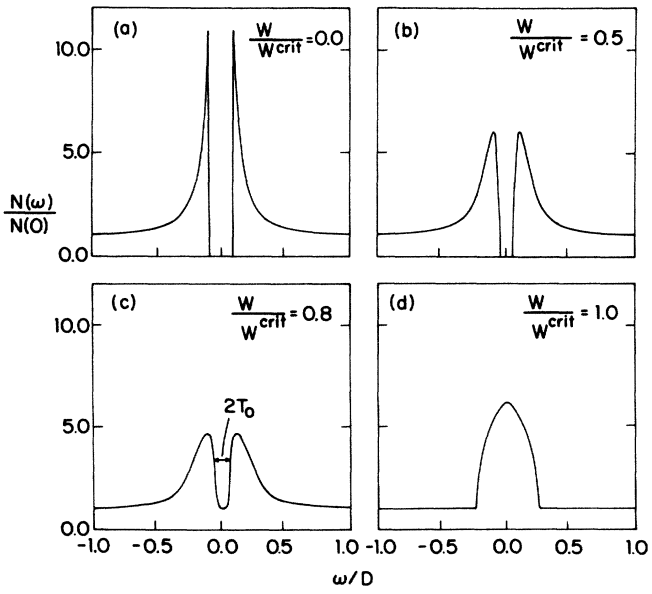


FIG. 2. Dynamical quasiparticle density of states for various degrees of disorder. As explained in the text we choose $(D/T_K)=10$.

that the coherence temperature $T_0$ is a quantity critically dependent on the purity, structural defects, and other material characteristics of a given sample.

We interpret these results as indicating that, above a certain concentration, the impurities prevent formation of the heavy band. Heavy-fermion materials in which the disorder exceeds the critical value are expected to show a smooth crossover to the concentrated Kondo impurity behavior lacking the characteristic signatures of coherence in low-temperature resistivity, specific heat, etc. To further clarify this note that $b_i$ is a local field, the similar mean-field solution exists for the single impurity problem.[9] Our approximate treatment of the random scattering was based on the assumption that the average value of the $b$ field is much larger than its rms fluctuations. For a disorder approaching the critical value this will no longer be the case and one will have to consider the spatial variations of $b_i$ and $\lambda_i$. These variations will tend to adjust to the local impurity configuration, leading to behavior increasingly similar to that of independent Kondo moments. This would tend to increase our mean-field estimate of $W^{\rm crit}$. The upper bound for $W^{\rm crit}$ seems to be given by $V^2/D$, so we can conclude, in general, $T_k \lesssim W_f^{\rm crit} < V^2/D$.[13] $W^{\rm crit}$ sets the overall scale at which the crossover from the Kondo lattice to the concentrated Kondo impurity system. One should note at this point that, while the disorder strongly affects the coherent behavior, the thermodynamics is expected to change very little. This is the consequence of the Kondo temperature $T_K$ still setting the overall energy scale, as one can see from Fig. 1(d).

The above conclusions seem to be supported by experiment.[14] Very low concentrations of impurities in $UBe_{13}$ lead to depression of the coherence peak in resistivity to lower temperatures and to an increase in its residual value. Ultimately, resistivity shows a monotonic, sharp rise as the temperature is reduced, indicative of a loss of carriers. This is clearly in accord with our conclusions concerning the breakdown of the heavy band. Similar features have been observed in experiments with other heavy-fermion systems.[12] A common way of disordering heavy-fermion materials is through substitution of Ce or U by their neighbors in the periodic system which do not have $f$ electrons (for example La or Lu). In the lowest order approximation we can model this situation by setting the hybridization matrix element $V$ to zero at impurity sites. Within our SCBA scheme the "critical" concentration $c$ necessary to destroy coherence is then $\simeq 50\%$; similarly if one applies the coherent potential approximation (CPA) to the same problem, $c = 33\%$. These high values for $c$ are not surprising since modeling the effect of impurities by only setting $V=0$ at appropriate sites completely ignores the "Kondo volume collapse".[14] Impurity atoms cause significant local changes in the volume of the unit cell accompanied by strong internal stresses. The characteristic pressures involved are typically of order $\simeq 10-10^2(T_K/\Omega_0)$, where $\Omega_0$ is the unit-cell volume.[15,16] If we represent these internal stresses by randomly varying potential the critical concentration is brought down to $1-10\%$. This clearly indicates the importance that the Kondo volume collapse and impurity size effects have for coherence and is particularly significant in the context of our result that scattering on the $f$ sites is more important than on $c$ sites. On a qualitative level, we predict that the critical concentration will be smaller for large impurity atoms, like La or Lu, which tend to occupy Ce or U sites, rather than for small atoms which will preferably occupy sites of a host metal (Be, Pt, or Cu). For more direct comparison with experiment, however, realistic models for the matrix $W$ are required dealing with the specific impurity atoms in a given compound; work is in progress along these lines.[17]

In summary, we have presented the first study of the effects of disorder on the coherent heavy band formation in heavy-fermion materials. Our results indicate that the disorder strongly affects coherence, and correspondingly may induce significant changes in the effective interactions between the heavy fermions. The Kondo volume collapse and the impurity size effects appear to be quantitatively dominant factor in suppressing the formation of the heavy band. For disorder close to the critical value we expect that the spatial variations in $b$ become very important; formulating the description in which these variations are taken into account and therefore obtaining a more detailed understanding of the "crossover" between the Kondo lattice and the collection of single impurities would be a natural extension of this work.

## ACKNOWLEDGMENTS

The author is grateful to P. A. Lee, G. B. Kotliar, T. M. Rice, R. M. Martin, D. Pines, D. Rainer, and A. J. Millis for comments and critical remarks. This work has been supported in part by the National Science Foundation (NSF) through Grant Nos. DMR-82-07431 and MPS-85-14638 and the Harvard University Materials Research Laboratory.

[1]H. R. Ott, H. Rudigier, Z. Fisk, and J. L. Smith, Phys. Rev. Lett. **50**, 1595 (1983).

[2]W. Lieke, U. Rauchschwalbe, C. D. Bredl, and F. Steglich, J. Appl. Phys. **53**, 2111 (1982); U. Rauchschwalbe, W. Lieke, C. D. Bredl, F. Steglich, J. Aarts, K. M. Martini, and A. C. Mota, Phys. Rev. Lett. **49**, 1448 (1982).

[3]G. R. Stewart, Z. Fisk, J. O. Willis, and J. L. Smith, Phys. Rev. Lett. **52**, 679 (1984).

[4]For review see, P. A. Lee, T. M. Rice, J. W. Serene, L. J. Sham, and J. W. Wilkins, Comments Solid State Phys. (to be published).

[5]For review see, G. R. Stewart, Rev. Mod. Phys. **56**, 755 (1984).

[6]K. Wilson, Rev. Mod. Phys. **47**, 773 (1975)

[7]N. Andrei, K. Furuya, and J. Lowenstein, Rev. Mod. Phys. **55**, 331 (1984).

[8]For papers particularly relevant to the heavy-fermion problem the reader should consult Ref. 4. The most recent work includes T. M. Rice and K. Ueda, Phys. Rev. Lett. **55**, 995 (1985); C. M. Varma and A. Zawadowski, Phys. Rev. B **32**, 7399 (1985); C. M. Varma, W. Weber, and L. J. Randall, *ibid.* 1015 (1986); N. Read and D. M. Newns, Solid State Commun. **52**, 993 (1984); and B. Brandow, Phys. Rev. B **33**, 215

(1986).

[9]N. Read and D. M. Newns, J. Phys. C **16**, 3273 (1983); P. Coleman, Phys. Rev. B **29**, 3035 (1984); N. Read, D. M. Newns, and S. Doniach, *ibid.* **30**, 3841 (1984).

[10]P. Coleman, Institute for Theoretical Physics (University of California, Santa Barbara) Report No. ITP-91 (1986) (unpublished).

[11]In fact, this result is just an example of the considerable importance that the difference in spectral weights has in determining the effects of impurity scattering. It is interesting to note that in a hypothetical BCS superconductor, in which the Cooper pairs are formed *only* between two different species of electrons, say $s$ and $d$, even nonmagnetic impurities have a pair-breaking effect.

[12]C. D. Bredl, S. Horn, F. Steglich, B. Luthi, and R. M. Martin, Phys. Rev. Lett. **52**, 1982 (1984).

[13]T. M. Rice and K. Ueda (to be published). I thank T. M. Rice for a discussion of this point.

[14]H. R. Ott, H. Rudigier, E. Felder, Z. Fisk, and J. L. Smith, Phys. Rev. B **33**, 126 (1986).

[15]J. W. Allen and R. M. Martin, Phys. Rev. Lett. **49**, 1106 (1982).

[16]H. Razafimandimby, P. Fulde, and J. Keller, Z. Phys. B **54**, 111 (1984).

[17]Z. Tešanović (unpublished).