Stability of the Kondo lattice in the large-N limit

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We consider a Kondo lattice of rare-earth ions, as a description of materials such as YbCuAl and α-Ce, by an expansion in $1/N$, where $N=2j+1$. We show that in the large-N limit the nonmagnetic state is stable against magnetic order and that its susceptibility and specific heat are those of an ensemble of isolated impurities.

I. INTRODUCTION

In recent work using a steepest-descent approach, Read and Newns[1] have shown that the low-temperature properties of a magnetic impurity with one f electron occupying N degenerate levels coupled to a Fermi sea [the Coqblin-Schrieffer or SU(N) Kondo model[2]] may be represented by a suitably renormalized noninteracting resonant level model in the limit of large N. This follows earlier suggestions[3] that the Kondo problem should have a simple expansion in powers of $1/N$. The results of this approach for properties involving low-lying excitations of the system (specific heat, susceptibility) are in accord with exact solutions of the N-level problem using the Bethe ansatz.[4]

In this paper we show that a similar limit may be taken for the Kondo lattice, a periodic lattice of singly occupied identical N-level ions interacting with a Fermi sea via a Coqblin-Schrieffer coupling. We find that in the large-N limit, the ground-state energy and low-temperature thermodynamic properties of the nonmagnetic state of the Kondo lattice become those that the individual ions would have if they were dilute impurities, so that they only feel each others presence to order $1/N$. As a consequence of this property, we show that the critical value of the coupling constant J_0 above which the nonmagnetic state remains stable (introduced by Doniach[5] and Jullien *et al.*[6] for the spin-$\frac{1}{2}$ case) goes to zero as $N\to\infty$. This result follows from a comparison of the ground-state energy of the nonmagnetic Kondo state of the lattice with that of a magnetic state of the lattice calculated using the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction induced by the spin—conduction-electron coupling.

II. COMPUTATION OF THE LARGE-N LIMIT BY STEEPEST DESCENT

Our starting point is the Coqblin-Schrieffer[2] [or SU(N) Kondo] model, generalized to a lattice:

$$H=\sum_{\vec{k}}\epsilon_{\vec{k}}c^{\dagger}_{\vec{k}}c_{\vec{k}}-\frac{J_0}{N}\sum_{i,M,M'}f^{\dagger}_{iM}c_{iM}c^{\dagger}_{iM'}f_{iM'}\ , \tag{1a}$$

where

$$c^{\dagger}_{iM}=\sum_{\vec{k}}(4\pi)^{1/2}[Y^M_L(\Omega_{\vec{k}})]^* e^{-i\vec{k}\cdot\vec{R}_i}c^{\dagger}_{\vec{k}}\ , \tag{1b}$$

and $f^{\dagger}_{iM}$ creates an f electron at site i in angular momentum channel M; it is understood that $n_{fi}=1$. In this paper we have for simplicity treated only spinless electrons and neglected spin-orbit coupling, so that M runs from $-L$ to L giving the degeneracy of our f states as $N=2L+1$. Inclusion of spin and of the Clebsch-Gordan coefficients restores the correct degeneracy $N=2j+1=2l+1\pm1$, but does not affect the essentials of our argument.

To find the large-N limit in the nonmagnetic regime we decouple (1) by a Stratonovich-Hubbard transformation for the partition function, as in Ref. 1, and calculate properties of the ground state. Thus

$$Z=\mathrm{Tr}\int D\phi\, D\lambda \exp\left[-\int_0^{\beta}H_{\mathrm{eff}}[\phi,i\lambda]d\tau - \frac{N}{J_0}\sum_i\int_0^{\beta}\phi_i^2(\tau)d\tau\right], \tag{2}$$

where

$$H_{\mathrm{eff}}=\sum_{\vec{k}}(\epsilon_{\vec{k}}-\mu)c^{\dagger}_{\vec{k}}c_{\vec{k}}+\sum_{i,M}\phi_i(\tau)(f^{\dagger}_{iM}c_{iM}+c^{\dagger}_{iM}f_{iM}) +i\sum_i\lambda_i(\tau)\left[\sum_M f^{\dagger}_{iM}f_{iM}-1\right], \tag{3}$$

and the term in $\lambda_i(\tau)$ which fixes the number of f electrons per site at unity originates via a gauge transformation from the phase of the (originally complex) ϕ field.[1]

In Ref. 1 it was found that low-temperature properties in the single impurity problem could be calculated to lead-

ing order in $1/N$ by a steepest-descent method, replacing $\phi(\tau)$ and $i\lambda(\tau)$ in (3) by constant values ϕ_0 and $\epsilon_f-\mu$ (which are chosen to minimize the effective free energy which results when the fermion trace has been taken) and neglecting fluctuations in $\phi-\phi_0$ and λ. Then ϵ_f becomes the renormalized position of the f level, chosen to fix the f occupation at one per site, and ϕ_0 becomes an effective hybridization between f and band states. We follow this procedure here to find the properties of a translationally invariant ground state in which ϵ_f and ϕ_0 are the same on each lattice site.

It follows that to compute ground-state properties we only need to solve the hybridized band-structure problem[7] of diagonalizing $H_{\rm eff}[\phi_0,\epsilon_f-\mu]$ given in (3) and then determining ϵ_f, ϕ_0, and μ self-consistently (the chemical potential μ is determined by fixing the number of electrons in the conduction band). This problem is, however, greatly simplified to leading order in $1/N$ as follows: We define the (diagonal) retarded propagators $G_{fc}(\epsilon)$ and $G_{ff}(\epsilon)$ as the Fourier transforms of

$$-i\langle Tf_{iM}(t)c^{\dagger}_{iM}(0)\rangle\Theta(t)$$

and

$$-i\langle Tf_{iM}(t)f^{\dagger}_{iM}(0)\rangle\Theta(t)\ ,$$

respectively. These can be calculated perturbatively starting from $H_{\rm eff}[\phi_0,\epsilon_f-\mu]$ once we realize that we need only their values at energies below the Fermi level μ, and that $\phi_0^2\rho_0\simeq(\epsilon_f-\mu)/N$, as justified below ($\rho_0$ is the density of conduction band states near $\epsilon=\mu$), so that the perturbation on states below the Fermi level is weak. So for G_{fc},

$$G_{fc}(\epsilon+i\delta)=\frac{1}{\epsilon-\epsilon_f+i\delta}\phi_0 g_{MM}(\vec{0},\epsilon)+\frac{1}{\epsilon-\epsilon_f+i\delta}\phi_0\sum_{\vec{R},M'}g_{MM'}(-\vec{R},\epsilon)\frac{\phi_0^2}{\epsilon-\epsilon_f+i\delta}g_{M'M}(\vec{R},\epsilon) \tag{4}$$

plus higher-order terms involving 3,4,5,... sites. Here the propagator

$$g_{MM'}(\vec{R}_i-\vec{R}_j,\epsilon)=\sum_{\vec{k}}\frac{4\pi Y_L^M(\Omega_{\vec{k}})[Y_L^{M'}(\Omega_{\vec{k}})]^*}{\epsilon-\epsilon_{\vec{k}}+i\delta}\times e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)} \tag{5}$$

takes an electron from partial-wave state M' at site j to state M at site i. Now if for fixed $\vec{R}$ we take angular momentum states quantized around $\vec{R}$, we find that $g_{MM'}(\vec{R},\epsilon)$ is diagonal in M and M' and of order N^0 in each channel. Hence in the two-site term in (4) we have shown that the sum over $\vec{R}$ and M contributes no additional factor N, so that the term is $O(1/N)$ smaller than the preceding single-site term. Similarly all multisite terms must be at least $O(1/N)$ compared with the single-site term. This single-site term, and the similar one for G_{ff}, involve the sum

$$g_{MM}(\vec{0},\epsilon)=\sum_{\vec{k}}(\epsilon-\epsilon_{\vec{k}}+i\delta)^{-1}$$

whose imaginary part just gives the local density of states ρ_0 for the conduction band.

The ground-state energy can now be calculated from the coupling-constant integral for the one-electron energy contribution E^1,

$$E^1=2N\int_0^{\phi_0}d\phi_0\int^{\mu}d\epsilon\left[-\frac{1}{\pi}\mathrm{Im}G_{fc}(\epsilon+i\delta)\right]$$

$$\simeq N\rho_0\phi_0^2\ln[(\epsilon_f-\mu)/D]\ , \tag{6}$$

where we have used the local leading contribution to G_{fc}, just derived, taken the density of states in the band as approximately flat near $\epsilon=\mu$ and D is the energy difference between μ and the effective bottom of the conduction band (it is assumed that $\epsilon_f-\mu\ll D$). The change in energy due to switching on the coupling ϕ_0 is then

$$\Delta E_0=N\rho_0\phi_0^2\ln[(\epsilon_f-\mu)/D]-(\epsilon_f-\mu)+\frac{N}{J_0}\phi_0^2\ . \tag{7}$$

As discussed above, we require that ΔE_0 be stationary with respect to variations in ϵ_f and ϕ_0, giving

$$N\rho_0\phi_0^2=\epsilon_f-\mu\ ,\quad \epsilon_f-\mu=D\exp(-1/\rho_0 J_0)\equiv T_K\ , \tag{8}$$

which self-consistently justify our assumption that $\rho_0\phi_0^2$ is $O(N^{-1})$. The ground-state energy per rare-earth site of the Kondo lattice in the large-N limit is therefore

$$\Delta E_0=-T_K\ , \tag{9}$$

so that the total ground-state energy is precisely that which would be obtained by treating each ion as a dilute impurity.

III. PROPERTIES OF THE NONMAGNETIC GROUND STATE

The propagator G_{ff} is calculated similarly to G_{fc}, giving for the leading part of the local f density of states the single-site term

$$\rho_f(\epsilon)\simeq\phi_0^2\rho_0/(\epsilon-\epsilon_f)^2$$

in each channel M at or below the Fermi level. Hence, restoring the correct degeneracy factors, the zero-field susceptibility χ_0 at $T=0$, and linear coefficient γ of specific heat are given by ($N=2j+1$)

$$\chi_0=\tfrac{1}{3}j(j+1)g^2\mu_B^2/T_k\ ,$$
$$\gamma=\tfrac{1}{3}\pi^2k_B^2/T_k\ , \tag{10}$$

where we have used (8) and so their ratio is

$$\frac{\chi}{\gamma}=\frac{j(j+1)\mu_B^2}{\pi^2k_B^2}\left[1+O\left[\frac{1}{N}\right]\right]\ . \tag{11}$$

The $O(1/N)$ corrections are here due both to intersite one-electron effects and to fluctuation corrections.[1] Equations (8) to (11) are the same results as were found in the single impurity case in the large-N limit. Thus thermodynamic properties of the nonmagnetic (Kondo) ground state of the Kondo lattice in the large-N limit are those of independent impurities, although the exact eigenstates of $H_{\rm eff}[\phi_0,\epsilon_f-\mu]$ are of course Bloch waves as would be seen in studies of transport phenomena, excitation spectrum, etc.

The same results have also been obtained in a more simplified model in which M is a good quantum number for the conduction band, so that

$$g_{MM'}(\vec{\mathrm{R}},\epsilon)=\delta_{MM'}g(\vec{\mathrm{R}},\epsilon)=\delta_{MM'}\sum_{\vec{\mathrm{k}}}\frac{e^{i\vec{\mathrm{k}}\cdot\vec{\mathrm{R}}}}{\epsilon-\epsilon_{\vec{\mathrm{k}}}+i\delta}\ ,$$

and the model consists of N degenerate, independent, hybridizing f, and conduction bands. This model can be diagonalized exactly (when $N=2$ it is similar to that of Lacroix and Cyrot[8]) and yields the same results found more generally above.

IV. COMPARISON WITH THE MAGNETIC GROUND STATE

To estimate the stability of the nonmagnetic ground state we compare (9) with the energy of a ground state which is fully magnetized via the version of the RKKY interaction appropriate for the Coqblin-Schrieffer model.[2,9] The second-order perturbation-theory formula for the interaction between two ions at a separation $\vec{\mathrm{R}}$ given in Ref. 2 can be written, with

$$\chi^{(i)}_{MM'}=f^\dagger_{iM}f_{iM'}-\frac{1}{N}\delta_{MM'}\sum_{M''}f^\dagger_{iM''}f_{iM''}\ ,$$

in the form

$$H_{ij}(\vec{\mathrm{R}})=\sum_{M,M'}E^{MM'}(\vec{\mathrm{R}})\chi^{(i)}_{MM'}\chi^{(j)}_{MM'}\ , \tag{12a}$$

$$E^{MM'}(\vec{\mathrm{R}})=\frac{J_0^2}{N^2}\left[-\frac{1}{\pi}\mathrm{Im}\int^\mu g_{MM}(\vec{\mathrm{R}},\epsilon)g_{M'M'}(-\vec{\mathrm{R}},\epsilon)d\epsilon\right]\ , \tag{12b}$$

with angular momentum quantized around $\vec{\mathrm{R}}$ once again. We note that the large-N limit is most appropriately taken with $\vec{\mathrm{R}}$ fixed and $L\to\infty$, not using the asymptotic formulas of Ref. 9, which are strictly valid only for impracticably large values, $|\vec{\mathrm{R}}|\gg L(L+1)k_c^{-1}$ (here k_c is a momentum cutoff of order N^0). An estimate of the lowest possible magnetic energy based upon each bond having the f state $M=0$ occupied is then [using the fact that g_{00} is largest and $O(N^0)$]

$$\Delta E_{\rm mag}\propto -J_0^2\rho_0^2D/N^2\ , \tag{13}$$

the constant of proportionality depending on the band structure and type of magnetic order. Therefore, for large N the Kondo ground state is stable provided $|\Delta E_0|>|\Delta E_{\rm mag}|$, or

$$\exp\left[\frac{-1}{\rho_0J_0}\right]>\frac{A(\rho_0J_0)^2}{N^2}\ , \tag{14}$$

where A is a constant independent of N, in agreement with the result of Coleman.[10] This implies that the critical coupling required to satisfy (14) vanishes as $N\to\infty$ as $J_0\rho_0\propto(2\ln 2N)^{-1}$ or that the smallest possible renormalization factor is

$$T_K/D\propto(2N\ln 2N)^{-2} \tag{15}$$

which lies in the region 10^{-3}–10^{-4}. Thus T_K/D can be very small for large N, and we can understand the strongly renormalized nonmagnetic ground states found in concentrated nearly integral-valent systems such as YbCuAl, where $N=8$, in which $T_K\simeq 8$ meV.[3] Similarly we can understand the fact that α-Ce (with many Ce compounds) has a nonmagnetic ground state[11,12] and can estimate its ground-state energy from (9) and (10) together with specific-heat and susceptibility data[3] as $\Delta E_0\simeq -150$ meV, rather larger than the estimate of 60 meV needed for the Kondo collapse theory.[11]

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[1] N. Read and D. M. Newns, J. Phys. C **16**, 3273 (1983).

[2] B. Coqblin and J. R. Schrieffer, Phys. Rev. **185**, 847 (1969).

[3] D. M. Newns and A. C. Hewson, J. Phys. F **10**, 2429 (1980); and in *Valence Fluctuations in Solids*, edited by L. M. Falicov, W. Hanke, and M. B. Maple (North-Holland, Amsterdam, 1981), p. 27; T. V. Ramakrishnan and K. Sur, Phys. Rev. B

26, 1798 (1982); in *Valence Fluctuations in Solids,* p. 13; P. W. Anderson, *ibid.* p. 451.

[4]A. M. Tsvelick and P. B. Wiegmann, J. Phys. C **15,** 1706 (1982); J. W. Rasul, *Proceedings of the International Conference on Valence Instabilities,* edited by P. Wachter and H. Boppart (North-Holland, Zurich, 1982).

[5]S. Doniach, Physica (Utrecht) **91B,** 231 (1977).

[6]R. Jullien, J. Fields, and S. Doniach, Phys. Rev. B **16,** 4889 (1977); R. Jullien, P. Pfeuty, and B. Coqblin, *Valence Fluctuations in Solids,* edited by L. M. Falicov, W. Hanke, and M. E. Maple (North-Holland, Amsterdam, 1981), p. 169.

[7]S. Doniach, in *The Actinides,* edited by A. J. Freeman and J. B. Darby (Academic, New York, 1974), Vol. II. p. 51.

[8]C. Lacroix and M. Cyrot, Phys. Rev. B **20,** 1969 (1979).

[9]R. Siemann and B. R. Cooper, Phys. Rev. Lett. **44,** 1015 (1980).

[10]P. Coleman, Phys. Rev. B **28,** 5255 (1983).

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

[12]M. Lavagna, C. Lacroix, and M. Cyrot, J. Phys. F **13,** 1007 (1983).