$1/N$ expansion for the f^1-f^2 Anderson model: Wilson ratio, Fermi-liquid relations, and charge-fluctuation energies

J. W. Rasul
The Department of Physics, The University of Michigan, Ann Arbor, Michigan 48109-1120
(Received 27 December 1989)

We calculate the $1/N$ correction to the free energy of the f^1-f^2 Anderson model (where N is the spin-orbit degeneracy of Tm or Pr impurities in a metal). We obtain the $1/N$ correction to the Wilson ratio (χ/γ) and relate this to the zeroth-order charge susceptibility. We find the Yoshimori-Schlottmann Fermi-liquid relation is satisfied to this order in $1/N$. The charge-fluctuation energy scales obtained by expressing the results in universal form agree with earlier scaling theories.

I. INTRODUCTION

Interest in the correlated electron problem has flourished over the past few years in many contexts: high-T_c systems, the metal-insulator transition, heavy fermions, and valence fluctuators. The latter two fields have led people to study dilute-magnetic-impurity problems as a first step towards understanding the many-body renormalizations occurring in lattice models. Even though exact numerical renormalization-group[1] and Bethe-ansatz[2] solutions have been available, the challenge has been to describe the magnetic-impurity problem adequately within a many-body treatment that can be treated as input for (or in competition with) lattice theories.

The impurity Anderson model provides a convenient framework for studying the range of fluctuating-valence to local-moment behavior. For Ce or Yb impurities in which the local state fluctuates between a magnetic $f^1(f^{13})$ and a nonmagnetic $f^0(f^{14})$ configuration a number of reasonable many-body treatments have been developed, and in recent years a lot of attention has been focused on the $1/N$ expansion[3] (where N denotes the spin-orbit degeneracy).

For the case where the two lowest atomic configurations both are degenerate, a lot less work has been done. Where crystal fields are such as to produce nonmagnetic doublets, the dominant fluctuations are expected to be quadrupolar.[4] However, if both configurations carry magnetic moments, different physics is involved. Variational studies of the f^1-f^2 Anderson model by Yafet *et al.*[5] showed that hybridization produced a many-body singlet ground state, in which the f^1 and f^2 components of the wave function contained in addition one and two holes, respectively, thereby screening the overall moment. Furthermore, the energy scale separating this singlet from higher magnetic states was found to be very small, typically of the order of a Kondo temperature, even with the valence well in between the f^1 and f^2 limits. The f^1-f^2 problem was treated by Read, Dharmvir, Rasul, and Newns[6] (hereafter referred to as RDRN) using a $1/N$ expansion and similar conclusions were reached. A singlet ground state and small intermediate-valent energy scale were also obtained for the f^2-f^3 Anderson model, perhaps a suitable starting point for dilute uranium systems.[7] The variational method has been extended to the calculation of the magnetic response of the f^1-f^2 model.[8] More recently the noncrossing approximation (NCA) has been formulated for this problem[9] and a numerical renormalization-group (RG) study[10] has confirmed that the ground state is a many-body singlet of the type discussed earlier.

In this paper we extend the $1/N$ expansion procedure formulated by RDRN in an effort to obtain reasonable quantitative results for the low-temperature properties of the f^1-f^2 Anderson model. Although this expansion procedure requires we use a highly simplified model, namely a j-j–coupling model in the limit of zero j-j coupling, the recent RG results imply that the $1/N$ expansion even at leading order reproduces the correct physics and hence provides a good starting point. Furthermore, experience with the Kondo problem has shown that the $1/N$ expansion constitutes the only reliable guide for reordering perturbation theory so as to obtain nondivergent results at low temperatures.[3] If the correct low-temperature behavior of this model can be obtained, the formalism can then readily be applied to more realistic coupling schemes.

In particular we calculate the quasiparticle energy of the singlet state to next-leading order in $1/N$ and obtain the $1/N$ correction to the Wilson ratio χ/γ. Such a systematic $1/N$ perturbation procedure[11] is known to yield accurate results for the f^0-f^1 problem (where exact Bethe-Ansatz results are available) for the susceptibility, valence, crossover number $W(N)$, and also the χ/γ ratio.[3] In contrast the NCA, while providing a good overall description as a function of temperature, has nonanalyticity in the Fermi-liquid regime. The slave boson method[12] of particular convenience for the f^0-f^1 problem, when formulated in spinless terms,[13] does not recover the $1/N$ limit correctly. Spin-carrying tensor bosons are required in this case[12] and do not appear to simplify this problem to the extent the boson method does in the f^0-f^1 case.

We start from the f^1-f^2 Anderson model (spin j)

 ©1990 The American Physical Society

$$H=\sum_{\substack{m=-j\\k}}^{j}\varepsilon_{km}c_{km}^{\dagger}c_{km}+V\sum_{k,m}(|1m\rangle\langle 2mm'|c_{km'}^{\dagger}+c_{km'}|2mm'\rangle\langle 1m|)+E_1\sum_m|1m\rangle\langle 1m|+E_2\sum_{m,m'}|2mm'\rangle\langle 2mm'|+V_0\sum_{k,m}(c_{km}^{\dagger}|0\rangle\langle 1m|+|1m\rangle\langle 0|c_{km}) \quad (1)$$

[where ε_{km} denotes the conduction-electron energy (with spin m), V denotes the f^1-f^2 mixing element, and E_1,E_2 are the bare energies of the f^1 and f^2 configurations], to which an extra hybridization to the f^0 singlet state has been added. This allows use of the quasiparticle energy scheme used in RDRN to obtain diagrammatic expansions in powers of V for the singlet energy akin to a Brillouin-Wigner perturbation expansion. Although we take V_0 to zero at the end of the diagrammatic resummation in powers of $1/N$, the presence of the f_0 state allows us to reach a state which has the correct symmetry of the ground state. The quasiparticle energy scheme is adequate as long as we are dealing with low temperatures, and saves a lot of effort even at the $1/N$ level over other perturbative resummation schemes.[14]

In the next section we calculate the quasiparticle energy to next-leading order in $1/N$. In Sec. III we obtain expressions for the spin and charge susceptibilities ($\chi,\chi_{\rm ch}$) and specific-heat coefficient γ to leading order before extracting the $1/N$ correction to the Wilson ratio $R=\chi/\gamma$. We show that the Yoshimori-Schlottmann[15,16] relation between R and $\chi_{\rm ch}$ is satisfied to next-leading order in $1/N$. In Sec. IV we show that if we express our results in universal form, we obtain energy scales describing the charge fluctuations which agree with earlier scaling theories.

II. QUASIPARTICLE ENERGY TO NEXT-LEADING ORDER

In this section we recount the leading-order result of RDRN, generalized to include a magnetic field, and then proceed to discuss the $1/N$ corrections. Our basic quantity of interest is the f^0 singlet quasiparticle energy E_0, which results from adding to the f^1-f^2 Anderson model the extra hybridization term in Eq. (1). The diagrammatic procedure is then a straightforward generalization of the rules for the f^0-f^1 Anderson model;[6,17] the increasing time axis is taken from left to right, and the initial f^0 state is occupied by a band electron (with spin) at some time, with a matrix element V_0, and becomes vacant later, again with a matrix element V_0. The band-electron propagation is represented by a Fermi function $f(\varepsilon_m)$ where ε_m is the electron energy (spin) and the intermediate f^1 state contributes on energy denominator $E_{1m}-E_0-\varepsilon_m$. This constitutes the lowest-order process. The intermediate f^1 state can then be dressed to leading order in $1/N$ by an infinite number of f^1-f^2 processes in which another electron (with spin m') hops in and then out of the f state. This has the effect of renormalizing the f' energy denominator as follows:

$$E_{1m}-E_0-\varepsilon_m\to d_m(\varepsilon_m)=E_{1m}-E-\varepsilon_m-V^2\sum_{c',m'\neq m}\frac{f(\varepsilon',m')}{(E_{2mm'}-E_0-\varepsilon_m-\varepsilon_{m'})}, \quad (2)$$

where $E_{2mm'}-E_0-\varepsilon_m-\varepsilon_{m'}$ is the energy denominator for the intermediate f^2 state with two holes present. Once an intermediate f^2 state is created, however, another possibility is that the original (spin) electron hops into the band, so that the resulting f^1 state has changed spin. This procedure can continue indefinitely, still yielding contributions of leading order in the $1/N$ expansion as long as all the band lines are joined up to give only hole propagators (i.e., Fermi functions). The result of this procedure is illustrated in Fig. 1(a). As each successive hole line involves a different energy (and spin) the iteration procedure is most easily represented in terms of a vertex function $\alpha_m(\varepsilon_m)$. The quasiparticle energy is then given by

$$E_0=V_0^2\sum_{m,\varepsilon}\frac{f(\varepsilon_m)\alpha_m(\varepsilon_m)}{d_m(\varepsilon_m)}, \quad (3)$$

where the vertex function $\alpha(\varepsilon)$ satisfies the integral equation described in Fig. 1(b);

$$\alpha_m(\varepsilon_m)=1+V^2\sum_{\varepsilon_2,m'\neq m}\frac{f(\varepsilon_2,m')\alpha'_m(\varepsilon_2,m')}{d_m(\varepsilon_2)L(\varepsilon_1,\varepsilon_2,m',m)}, \quad (4)$$

where $L(\varepsilon,\varepsilon';m,m')=E_{2mm'}-E_0-\varepsilon_m-\varepsilon'_m$. The integral equations of RDRN,[6] and Yafet *et al.*,[5] can be obtained by setting $H=0$ and absorbing the renormalized f^1 energy denominator into the vertex function α, by introducing $\beta_m(\varepsilon_m)=\alpha_m(\varepsilon_m)/d_m(\varepsilon_m)$ and taking the $V_0\to 0$ limit in such a way that E_0 remains finite. This can be done by absorbing the factor V_0^2 into $\beta_m(\varepsilon_m)$ and letting V_0 tend to zero, after which the constant on the right-hand side (rhs) of (4) drops out and the quasiparticle energy is determined by the solutions of

$$d_m(\varepsilon_m)\beta_m(\varepsilon_m)=V^2\sum_{\varepsilon'}\sum_{m'\neq m}\frac{f(\varepsilon'_2,m')\beta_{m'}(\varepsilon'_{m'})}{L(\varepsilon,\varepsilon',m,m')}. \quad (5)$$

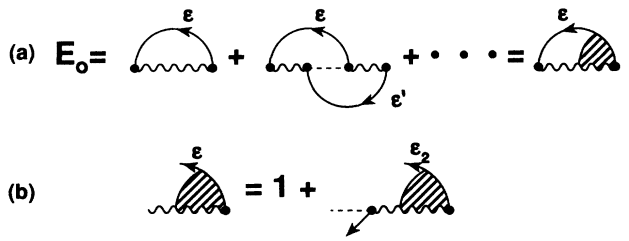

FIG. 1. (a) Diagrams for the singlet energy at leading order in terms of the vertex function $\alpha(\varepsilon)$. Wiggly lines denote the renormalized f^1 interval while dashed lines represent the bare f^2 state. Band electrons are represented by solid lines. (b) Integral equation for the vertex function $\alpha(\varepsilon)$.

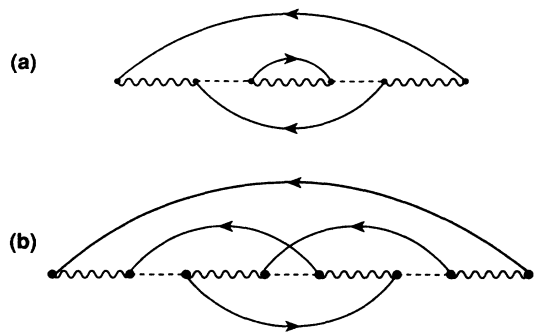

FIG. 2. Lowest-order diagrams in V^2 contributing to next-leading order in $1/N$.

The assumption of equal g factors for local and band electrons leads to the enormous simplification that the magnetic field cancels out in all energy denominators, since it appears with the same spin index equating in both band and local energies. The only place the field appears explicitly is then in the argument of the Fermi functions. Looking at (5) we see that at leading-order $1/N$ the restriction on the spin sum can be dropped, and the expansion at the Fermi function in the field leads to the appearance of only even powers of H. It is easy to see that the Sommerfeld expansion into terms at order T^2 will lead to the same expressions (apart from proportionality factors involving Boltzmann's constant and the electron g factors) as those obtained in the field expansion. The many-body processes involved at leading order in the $1/N$ expansion therefore enter identically into the calculation at χ and γ so that the Wilson ratio $R=\tilde{\chi}/\tilde{\gamma}$ [where $\chi=1/3j(j=1)\tilde{\chi}$ and $\gamma=\pi^2 k_\beta^2\tilde{\gamma}/3$] is equal to unity, as in the large-N limit of the f^0-f^1 Anderson model. However, we shall show later that at the next order in the $1/N$ expansion the spin-summation restriction in (4) becomes important for R. The origin of this restriction is the Pauli principle. As shown by Evans and Gehring[8] it forces the effective moment μ_{eff} to take different values in the two local-moment limits.

Turning now to the next-leading-order connections we recall that in the f^0-f^1 problem these are obtained by including conduction electron-hole processes. The simplest such diagram for the f^1-f^2 problem [illustrated in Fig. 2(a)] involves dressing an intermediate f^2 line with a conduction-electron f^1 bubble. Including the renormalization of the f^1 line (to leading order in $1/N$) and inserting the vertex function in the right-hand corner generates a set of diagrams contributing to order $1/N$.

Further $O(1/N)$ graphs are obtained by cutting the innermost f^1 interval and innermost hole propagator in Fig. 2(a) and inserting an f^2 interval. The hanging hole lines are connected to the two remaining f^1-f^2 vertices, producing the skeleton diagram shown in Fig. 2(b). The hole lines have distinct spin indices, so this diagram is at the same order in $1/N$ as Fig. 2(a). This insertion procedure can be extended *ad infinitum*. Clearly this development parallels the vertex-renormalization procedure occurring at leading order [Fig. 1(a)]—each insertion introduces an extra energy dependence—so an integral equation representation is expected.

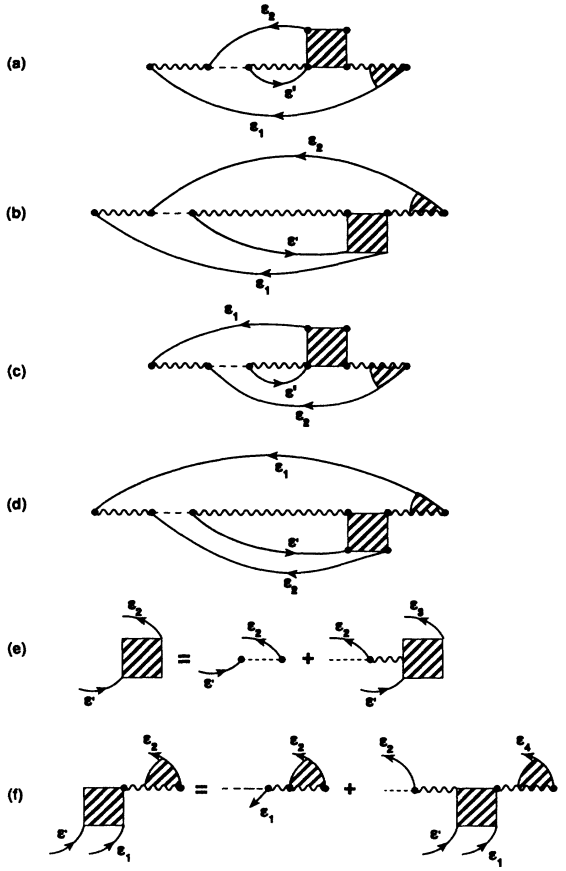

FIG. 3. (a)–(d) Next-leading-order contributions to E_0 in terms of the higher-order vertex functions M and $\tilde{M}$. Integral equations for these vertex functions are represented graphically in (e)–(f). The intervals between successive dots yield either $L(\Delta\varepsilon)$ or $d(\Delta\varepsilon)$ as explained in the text (where $\Delta\varepsilon$ involves the difference between leftward and rightward running energies). Lines with closed ends denote intermediate energies that are summed over.

We therefore introduce a function $M(\varepsilon_1,m:\varepsilon_2,m';\varepsilon',m)$ which satisfies

$$M(\varepsilon_1,m,\varepsilon_2,m':\varepsilon',m')=L(\varepsilon_1+\varepsilon_2)^{-1}+V^2\sum_{\substack{\varepsilon_3\\ m_3}}\frac{f(\varepsilon_3,m_3)M(\varepsilon_1,m,\varepsilon_2,m_3:\varepsilon' m)}{d(\varepsilon_1+\varepsilon_3-\varepsilon')L(\varepsilon_1+\varepsilon_3+\varepsilon_2-\varepsilon')}\ . \tag{6}$$

The contribution to E_0 from the series of diagrams in Figs. 2(a) and 2(b) can then be written

$$U^2V^4\sum_{\substack{\varepsilon_2\\ m}}\frac{f(\varepsilon_1,m)}{d(\varepsilon_1)^2}\sum_{\substack{\varepsilon'\\ \varepsilon_2\\ m'}}\frac{f(\varepsilon_2,m')[1-f(\varepsilon',m)]M(\varepsilon_1,m,\varepsilon_2,m':\varepsilon' m)\alpha(\varepsilon_1,m)}{L(\varepsilon_1+\varepsilon_2)d(\varepsilon_1+\varepsilon_2-\varepsilon')}\ , \tag{7}$$

which we represent diagrammatically in Fig. 3(a). As the overall contribution to E_0 from these diagrams is of order $1/N$ the spin-sum restrictions on internal-energy denominators may be ignored and consequently both $d(\varepsilon)$ and $L(\varepsilon)=E_2-E_0-\varepsilon$ are taken as independent of spin, whenever they appear in $O(1/N)$ graphs. Further $1/N$ diagrams are obtained by interchanging the ends of the outer two-hole lines in Fig. 3(a); interchanging the ends at these hole lines at the right-hand side produces the set of graphs represented in Fig. 3(b) which contribute to E_0 a term

$$U^2V^4\sum_{m,m'}\sum_{\substack{\varepsilon_1\\ \varepsilon_2\\ \varepsilon'}}\frac{f(\varepsilon_1,m)f(\varepsilon_2,m')[1-f(\varepsilon',m)]}{d(\varepsilon_1)d(\varepsilon_1+\varepsilon_2-\varepsilon')}\frac{\alpha_{m'}(\varepsilon_2)\tilde{M}(\varepsilon_1,m,\varepsilon_2,m':\varepsilon',m)}{L(\varepsilon_1+\varepsilon_2)}\ , \tag{8}$$

where $\tilde{M}(\varepsilon_1,m,\varepsilon_2,m';\varepsilon',m)$ satisfies the integral equation

$$\alpha(\varepsilon_3,m_3)\tilde{M}(\varepsilon_1,m_1,\varepsilon_3,m_3:\varepsilon',m_1)=\frac{\alpha(\varepsilon_3,m_3)}{d(\varepsilon_3)L(\varepsilon_1+\varepsilon_3)}+V^2\sum_{\substack{\varepsilon_4\\ m'}}\frac{f(\varepsilon_4,m')\tilde{M}(\varepsilon_1,m_1,\varepsilon_4,m':\varepsilon',m_1)\alpha_{m'}(\varepsilon_4)}{L(\varepsilon_1+\varepsilon_3+\varepsilon_4-\varepsilon')d(\varepsilon_1+\varepsilon_4-\varepsilon')}\ . \tag{9}$$

Interchanging the hole lines at the left-hand side (lhs) of Fig. 3(a) and swapping dummy indices yields a term

$$U^2V^4\sum_{\substack{\varepsilon_1,m\\ \varepsilon_2,m'}}\frac{f(\varepsilon_1,m)f(\varepsilon_2,m')}{d(\varepsilon_1)d(\varepsilon_2)}\frac{[1-f(\varepsilon',m')]\alpha(\varepsilon_2,m')}{L(\varepsilon_1+\varepsilon_2)d(\varepsilon_1+\varepsilon_2-\varepsilon')}M(\varepsilon_2,m',\varepsilon_1,m:\varepsilon' m') \tag{10}$$

illustrated in Fig. 3(c); while the same procedure applied to Fig. 3(b) yields a contribution to E_0

$$U^2V^4\sum_{\substack{\varepsilon_1,m\\ \varepsilon_2,m'\\ \varepsilon'}}\frac{f(\varepsilon_1,m)f(\varepsilon_2,m')\alpha(\varepsilon_1,m)\tilde{M}(\varepsilon_2,m',\varepsilon_1,m:\varepsilon',m')}{d(\varepsilon_1)d(\varepsilon_1+\varepsilon_2-\varepsilon')L(\varepsilon_1+\varepsilon_2)} \tag{11}$$

illustrated in Fig. 3(d).

The set of diagrams in Fig. 3 still do not constitute the full set of diagrams contributing to E_0 to order $1/N$. We can show that they should be regarded as constituting renormalizations of the f^1 and f^2 intermediate states entering into the leading-order diagrams of Fig. 1. In particular Figs. 3(a) and 3(d) can be regarded as renormalizing the f^1 intermediate state as follows:

$$d(\varepsilon,m)\rightarrow\tilde{d}(\varepsilon,m)=d(\varepsilon,m)-V^4\sum_{\substack{\varepsilon_1\\ \varepsilon_2,m'}}\frac{f(\varepsilon_2,m')S(\varepsilon_2,m',\varepsilon_1,m:\varepsilon',m')}{L(\varepsilon_1+\varepsilon_2)}\ , \tag{12}$$

and Figs. 3(b) and Fig. 3(c) renormalize the f^2 intermediate state

$$L(\varepsilon_1+\varepsilon_2)\rightarrow\tilde{L}(\varepsilon_1+\varepsilon_2)=L(\varepsilon_1+\varepsilon_2)\left[1-V^2\sum_{\varepsilon'}S(\varepsilon_1,m_1,\varepsilon_2,m_2:\varepsilon' m')\right]\ , \tag{13}$$

where $S(\varepsilon_1,m,\varepsilon_2,m':\varepsilon',m)$ is defined as follows:

$$S(\varepsilon_1,m,\varepsilon_2,m':\varepsilon',m)=\tilde{M}(\varepsilon_1,m,\varepsilon_2,m':\varepsilon',m)d(\varepsilon_2)\frac{[1-f(\varepsilon',m)]}{d(\varepsilon_1+\varepsilon_2-\varepsilon')}+\frac{M(\varepsilon_2,m',\varepsilon_1,m:\varepsilon',m')[1-f(\varepsilon',m')]}{d(\varepsilon_1+\varepsilon_2-\varepsilon')}\ . \tag{14}$$

Inserting these renormalizations into the f^1 and f^2 line to the left of the leading-order vertex function in Fig. 1(b) generates all the graphs in Figs. 2 and 3. Inserting these renormalizations into Eq. (5) we obtain after defining $\beta_m(\varepsilon_1)=\alpha_m(\varepsilon_1,m)/\tilde{d}(\varepsilon_1,m)$ the following integral equations for the quasiparticle energy:

$$\begin{aligned}d(\varepsilon_1,m)\beta_m(\varepsilon_1,m)-V^2\sum_{\varepsilon_2,m'\neq m}\frac{f(\varepsilon_2,m')\beta_{m'}(\varepsilon_2,m')}{L(\varepsilon_1+\varepsilon_2)}\\ =V^4\sum_{\substack{\varepsilon_1\\ m'\\ \varepsilon'}}\frac{f(\varepsilon_2,m')}{L(\varepsilon_1+\varepsilon_2)}\{[1-f(\varepsilon',m)]Q(\varepsilon_1,m,\varepsilon_2,m':\varepsilon',m)+[1-f(\varepsilon',m')]Q(\varepsilon_2,m',\varepsilon_1,m:\varepsilon',m')\}\ ,\end{aligned} \tag{15}$$

where Q satisfies

$$d(\varepsilon_1+\varepsilon_2-\varepsilon')Q(\varepsilon_1,m_1,\varepsilon_2{:}\varepsilon',m_1)=\frac{\beta(\varepsilon_1)+\beta(\varepsilon_2)}{L(\varepsilon_1+\varepsilon_2)}+V^2\sum_{\substack{\varepsilon_4\\ m_4}}\frac{f(\varepsilon_4,m_4)Q(\varepsilon_1,m_1,\varepsilon_4,m_4{:}\varepsilon',m_1)}{L(\varepsilon_1+\varepsilon_2+\varepsilon_4-\varepsilon')} . \tag{16}$$

These equations comprise the full set of $(1/N)$ diagrams for the f^1-f^2 model. They are equivalent to inserting processes of Fig. 3 at each interval in the diagrams shown in Fig. 1(a), and summing the resulting infinite set of diagrams.

III. $1/N$ CORRECTIONS TO THE WILSON RATIO χ/γ

In this section we calculate the $1/N$ correction to the Wilson ratio and show its relation to the zeroth-order change susceptibility χ_c. We obtain first expressions for χ, γ, and χ_c at leading order in $1/N$. We shall use the integral equation (5) with the spin restriction dropped, together with the zero-field, zero-temperature version of this equation

$$d_0(\varepsilon)\beta_0(\varepsilon)=\tilde{\Gamma}\int_{-D}^{0}d\varepsilon'\frac{\beta_0(\varepsilon')}{L_0(\varepsilon+\varepsilon')} , \tag{17}$$

where

$$d_0(\varepsilon)=E_1-E_{00}-\varepsilon-\tilde{\Gamma}\ln\frac{(D+E_2-E_{00}-\varepsilon)}{(E_2-E_{00}-\varepsilon)} ,$$

$$L_0(\varepsilon+\varepsilon')=E_2-E_{00}-\varepsilon-\varepsilon' ,$$

and

$$\tilde{\Gamma}=NV^2\rho_0 .$$

Here E_{00} is the ground-state energy to leading order in $1/N$, and ρ_0 is the conduction-band density of states at the Fermi level. We note that $\beta_0(\varepsilon)$ is unspecified up to an arbitrary factor. We shall determine this factor by the following argument. It was shown by RDRN that (17) is the same equation as that obtained by Yafet *et al.* for the amplitude of the f^1 conduction hole, and f^2 two-hole components at the ground-state wave function. In the $1/N$ language the ground-state wave function takes the form

$$|\psi\rangle_0=\sum_m\int_{-D}^{0}d\varepsilon\,\tilde{\beta}(\varepsilon)f_m^\dagger(\varepsilon)c_m(\varepsilon)|\text{F.s}\rangle+\sum_{m,m'}\int_{-D}^{0}d\varepsilon\int_{-D}^{0}d\varepsilon'\tilde{\gamma}(\varepsilon,\varepsilon')f_m^\dagger(\varepsilon)c_m(\varepsilon)f_{m'}^\dagger(\varepsilon')c_{m'}(\varepsilon')|\text{F.s.}\rangle , \tag{18}$$

where $\tilde{\beta}(\varepsilon)$ and $\tilde{\gamma}(\varepsilon,\varepsilon')$ are the amplitudes for the f^1 conduction hole and f^2 two-hole components, and $|\text{F.S.}\rangle$ denotes the filled Fermi sea. This state is a singlet and lies lower than any at the possible magnetic configurations at leading order in $1/N$. As long as $\tilde{\beta}(\varepsilon)$ is properly normalized, it is straightforward to show that the expectation value of the f occupation (the valence) is given by

$$\langle\psi|\sum_m f_m^\dagger f_m|\psi\rangle=n_f=2-\int_{-D}^{0}d\varepsilon\,\tilde{\beta}(\varepsilon)^2 . \tag{19}$$

Since (17) is a homogeneous integral equation we are free to fix the arbitrary-scale factor of $\beta_0(\varepsilon)$ so that $\beta_0(\varepsilon)$ and $\tilde{\beta}(\varepsilon)$ are equal. Then β_0 is the f^1 component of the wave function. Similarly, the finite-temperature equations (5), (15), and (16) may be scaled so that $\tilde{\beta}(\varepsilon)$ is the zero-temperature, zero-field limit of $\beta(\varepsilon)$ and that as $N\to\infty$ the quantity $\beta_m(\varepsilon)$ in Eq. (15) tends to this same function. This also fixes the amplitude $Q(\varepsilon_1,\varepsilon_2{:}\varepsilon')$. It should be noted that all these normalizations leave the quasiparticle energy E_0 unaffected.

Having determined the scale factors we return to Eq. (5), multiply by $\beta_0(\varepsilon)$, and then integrate over energy from $-D$ to 0, obtaining

$$\int_{-D}^{0}d\varepsilon\,d(\varepsilon)\beta(\varepsilon)\beta_0(\varepsilon)=\frac{1}{N}\sum_m\int_{-\infty}^{\infty}d\varepsilon'\beta(\varepsilon'_m)f(\varepsilon'_m)d_0(\varepsilon'+E_0-E_{00})\beta_0(\varepsilon'+E_0-E_\infty) . \tag{20}$$

The Sommerfeld expansion can now be performed, remembering that E_0-E_{00} is of order (H^2,T^2) and that $d(\varepsilon)$ itself has a series development in H^2 and T^2. After some manipulation we obtain (for $H=0$)

$$(E_0-E_{00})\int_{-D}^{0}d\varepsilon'\beta_0(\varepsilon')\beta_0'(\varepsilon')=-\pi^2\frac{k_B^2}{3}T^2q'(0)+O(T^4) , \tag{21}$$

where

$$q(\varepsilon)=d_0(\varepsilon)\beta_0(\varepsilon)^2+\tilde{\Gamma}\int_{-D}^{0}d\varepsilon'\frac{\beta_0(\varepsilon')^2}{L_0(\varepsilon+\varepsilon')} . \tag{22}$$

The same type of development can be carried out in powers of the field with the result that

$$(E_0-E_{00})\int_{-d}^{0} d\varepsilon'\beta_0(\varepsilon')\beta_0'(\varepsilon')=-\tfrac{1}{3}j(j+1)(g\mu_B)^2H^2q'(0)\ . \tag{23}$$

In terms of the quantities $\tilde{\chi}$ and $\tilde{\gamma}$ defined earlier the Wilson ratio is unity (as explained earlier) to leading order in $1/N$ because the Pauli-principle correction is negligible in this limit. Proceeding to the charge susceptibility we define a function $\beta_1(\varepsilon)$ equal to $d\beta_0/dE_{12}$ where $E_{12}=E_1-E_2$. This function describes the response at the f^1 amplitude to a charge in the relative positions at the bare f^1 and f^2 states. It is straightforward to show that $\beta_1(\varepsilon)$ satisfies the integral equation

$$d_0(\varepsilon)\beta_1(\varepsilon)-\tilde{\Gamma}\int_{-D}^{0} d\varepsilon'\frac{\beta_1(\varepsilon')}{L_0(\varepsilon+\varepsilon')}=-\beta(\varepsilon)-\alpha\, d(\varepsilon)\beta'(\varepsilon)\ , \tag{24}$$

where $\beta'(\varepsilon)$ denotes $(d/d\varepsilon)\beta(\varepsilon)$ and $\alpha=d(E_2-E_0)/dE_{12}$. It is useful at this stage to note that $\beta'(\varepsilon)$ satisfies the integral equation

$$d_0(\varepsilon)\beta'(\varepsilon)-\tilde{\Gamma}\int_{-D}^{0} d\varepsilon'\frac{\beta'(\varepsilon')}{L_0(\varepsilon+\varepsilon')}=2\,d(\varepsilon)\beta'(\varepsilon)-\Gamma(\beta(\varepsilon)+\beta(0))/(\delta-\varepsilon)-\beta(\varepsilon)\ , \tag{25}$$

which is obtained by differentiation of (17) followed by integration by parts. Multiplying (24) by $\beta_0(\varepsilon)$ and integrating over ε as before, the terms on the lhs vanish, so that

$$\int_{-D}^{0} d\varepsilon\, d(\varepsilon)\beta_0(\varepsilon)\beta_0'(\varepsilon)\alpha=-\int_{-D}^{0} d\varepsilon\,\beta_0(\varepsilon)^2\ . \tag{26}$$

Since α is simply equal to n_f-2 this relation is equivalent to

$$\int_{-D}^{0} d\varepsilon\, d_0(\varepsilon)\beta_0'(\varepsilon)\beta_0(\varepsilon)=1\ , \tag{27}$$

which is a restatement of the normalization condition. Integrating by parts we obtain $n_f=q(0)$. This relation can then be differentiated with respect to E_{12} to yield the charge susceptibility

$$\chi_{\rm ch}=\frac{dn_f}{dE_{12}}=2\,d(0)\beta(0)\beta_1(0)+[1+\alpha(1+\tilde{\Gamma}/\delta)]\beta(0)^2+2\int_{-D}^{0} dx\frac{\beta(x)}{(\delta-x)}\beta_1(x)-\alpha\int_{-D}^{0} dx\frac{\beta(x)^2}{(\delta-x)^2}\ , \tag{28}$$

where $E_2-E_{00}=\delta$. The susceptibility and specific heat are written concisely, to leading order in $1/N$ as $\tilde{\chi}=\tilde{\gamma}=q'(0)$.

We turn now to the $1/N$ corrections and follow the analysis of Bickers for the f^0-f^1 Anderson model.[3] At leading order in $1/N$ the singlet ground state is affected in the same way by either a magnetic field or an increase in temperature. Both bring into play excited band states through the single Fermi function in (5). Although the basic energy scale is determined by a nonlinear bound-state equation, the spectrum at this order is that of a free electron gas and the Wilson ratio is unity.

The $1/N$ correction break the symmetry between temperature and field, causing R to deviate from unity. The source of this difference is the low-energy behavior of the included equal-spin electron-hole pairs. The reason field and temperature couple differently to these states is that these states are bosonic at low energies. While these bosonlike energies do yield a T^2 contribution to the free energy, they do not couple to the magnetic field. We therefore have to extract this boson part.

We multiply (15) by the $N\to\infty$ limit of $\beta(\varepsilon)$ in Eq. (5) and integrate over energy as before. This yields the following expression:

$$\begin{aligned}-N\int d\varepsilon_1 f(\varepsilon_1)\beta(\varepsilon_1)\beta'(\varepsilon_1)\delta E_0=&-V^2\sum_m\int d\varepsilon_1 f(\varepsilon_1,m)\int d\varepsilon' f(\varepsilon',m)\frac{\beta(\varepsilon_1)[\beta(\varepsilon_1)+\beta(\varepsilon')]}{L(\varepsilon_1+\varepsilon')}\\&+V^4\sum_{m,m'}\int d\varepsilon_1 d\varepsilon_2 d\varepsilon'\frac{f(\varepsilon_1,m)f(\varepsilon_2,m')\beta(\varepsilon_1)}{L(\varepsilon_1+\varepsilon_2)}\\&\times\{[1-f(\varepsilon',m)]Q(\varepsilon_1,m,\varepsilon_2,m':\varepsilon' m)\\&+[1-f(\varepsilon',m')]Q(\varepsilon_2,m',\varepsilon_1,m.:\varepsilon',m')\}\ ,\end{aligned} \tag{29}$$

where δE_0 is the $1/N$ correction to the quasiparticle energy. We now extract the boson term by writing the electron-hole Fermi functions as follows:

$$f(\varepsilon_1,m)[1-f(\varepsilon',m)]=[f(\varepsilon',m)-f(\varepsilon_1,m)]b(\varepsilon_1-\varepsilon')\ , \tag{30}$$

where $b(\varepsilon)$ is the Bose function.

The remaining task is then to determine the low-energy behavior of the amplitude $Q(\varepsilon_1,\varepsilon_2:\varepsilon')$ for small $\varepsilon_1-\varepsilon'$, which is done by multiplying (16) by $\beta_0(\varepsilon)$ and integrating over ε. This leads to the relation

$$\tilde{\Gamma}\int d\varepsilon_2 d(\varepsilon_1+\varepsilon_2-\varepsilon')[\beta(\varepsilon_2)-\beta(\varepsilon_1-\varepsilon'+\varepsilon_2)]Q(\varepsilon_1,\varepsilon_2:\varepsilon')=q(\varepsilon_1)\ . \tag{31}$$

It follows that $Q(\varepsilon_1,\varepsilon_2:\varepsilon')$ is a singular function of $\varepsilon_1-\varepsilon'$ of the form

$$Q(\varepsilon_1,\varepsilon_2:\varepsilon')=-\frac{\beta(\varepsilon_2)q(\varepsilon_1)}{(\varepsilon_1-\varepsilon')}+\hat{Q}(\varepsilon_1,\varepsilon_2;\varepsilon')\ , \tag{32}$$

where $\hat{Q}(\varepsilon_1,\varepsilon_2:\varepsilon')$ is regular in $\varepsilon_1-\varepsilon'$, and satisfies an integral equation similar to (16) but with a different driving term. Making the replacement (30) in (29) requires that we know only the $\varepsilon_1=\varepsilon'=0$ limit of this function which satisfies

$$d_0(\varepsilon)\hat{Q}(0,\varepsilon:0)-\tilde{\Gamma}\int_{-D}^{0}d\varepsilon'\frac{\hat{Q}(0,\varepsilon';0)}{L_0(\varepsilon+\varepsilon')}$$
$$=(\beta(0)+\beta(\varepsilon))/L_0(\varepsilon)-(2+\alpha)d(\varepsilon)\beta'(\varepsilon)/\tilde{\Gamma}\ . \tag{33}$$

Comparing the driving terms of (33) with those in (24) and (25) we find that $\hat{Q}(0,\varepsilon:0)$ can be written in terms of $\beta_1(\varepsilon)$, $\beta'(\varepsilon)$, and $\beta(\varepsilon)$:

$$\hat{Q}(0,\varepsilon;0)=\frac{1}{\tilde{\Gamma}}[\beta_1(\varepsilon)-\beta'(\varepsilon)+q'(0)\beta(\varepsilon)/2]\ , \tag{34}$$

where the coefficient of $\beta(\varepsilon)$ is determined by substitution into (29).

The above expressions are sufficient to determine the bosonic contributions to δE_0. Substituting (34) and (32) into (29) and making use of (28) for the charge susceptibility χ_c we obtain after much algebra

$$-\delta E_0=1/(2N)[\chi_{\rm ch}-2\Gamma\beta(0)^2/\delta-q'(0)]\int_{-\infty}^{\infty}dy\,yb(y)\ , \tag{35}$$

describing the specific-heat correction from all $O(1/N)$ electron-hole-pair processes. To obtain the Wilson ratio to next-leading order in $1/N$ we have to include the Pauli-principle correction to χ/γ arising from the spin-sum restriction in Eq. (5). Combining these two effects leads to the cancellation of the second term in parentheses in Eq. (35), and we obtain finally the Wilson ratio to next-leading order in the $1/N$ expansion:

$$R=1+1/N-\chi_{\rm ch}/N\tilde{\gamma}\ . \tag{36}$$

The expression is the main result of this paper. It agrees to next-leading order in $1/N$ with the Fermi-liquid relation derived for the finite-U Anderson model by Yoshimori[15] for spin $\frac{1}{2}$ and extended to the degenerate case by Schlottman:[16]

$$\tilde{\gamma}=(N-1)/N\tilde{\chi}+1/N\chi_{\rm ch}\ . \tag{37}$$

This relation is basically a statement about the number of channels participating in the low-energy spectrum. One channel is due to the charge fluctuations and the remaining $N-1$ arise from the spin degrees of freedom. This result is not surprising in itself. In the present f^1-f^2 model, however, its formal derivation should require that one start from a finite-U Anderson model with an additional three-electron repulsion

$$U_3\sum_{m<m'<m''}\eta_m\eta_{m'}\eta_{m''}\ , \tag{38}$$

which is subsequently taken to infinity. Deriving the appropriate Ward identities in this case would then appear to be more complicated. This issue is left for further study.

We note that (35) has been invoked by Evans and Gehring[7] to estimate the variation of R with valence. By numerically differentiating the ground-state energy with respect to E_{12} they estimate the change of R due to $\chi_{\rm ch}$ to be a fraction of a percent. These authors include a single electron-pair correction to the f^2 self-energy.

IV. CHARGE FLUCTUATION ENERGY SCALES TO ORDER $1/N$

At the opposite end of the spectrum from the low-energy Fermi-liquid region are the charge-fluctuation energy scales. For Anderson-type models these scales are closely related to the ionic energy difference between f^1 and f^2 states, yet they also absorb all the essential dependence of physical quantities on the electron bandwidth. Since this dependence is logarithmic the simplest way to obtain these charge-fluctuation scales is via perturbative scaling.[18,19] As pointed out by Haldane[19] for the f^0-f^1 problem such a scale the crossover from valence fluctuation to local-moment behavior. For the f^1-f^2 case, RDRN showed that two such scales exist, one for each local-moment limit. They showed that the ground state, Eq. (5), could be written purely in terms of the singlet binding energy and the $N\to\infty$ limit of the charge-fluctuation energy scale, thereby removing the bandwidth D from the problem. We shall see how the charge-fluctuation scales enter at the $1/N$ level by focusing on the large-energy behavior of $Q(\varepsilon_1\varepsilon_2:\varepsilon')$ in Eq. (16). For large ε' this limiting behavior is simply found to be

$$Q(\varepsilon_1,\varepsilon_2:\varepsilon')=\frac{1}{(\varepsilon'-\varepsilon_1-\varepsilon_2)}\frac{(\beta(\varepsilon_1)+\beta(\varepsilon_2))}{(E_2-E_0-\varepsilon_1-\varepsilon_2)}\ , \tag{39}$$

so that the ε' integration on the rhs of (15) yields a term logarithmically dependent on the bandwidth. This term may, to $1/N$ order, be absorbed into the denominator of (15) which, apart from sublogarithmic $1/N$ corrections, becomes

$$(E_1-E-\varepsilon)\beta(\varepsilon)=(N-1)\Gamma_0\int_{-D}^{0}\frac{d\varepsilon'(\beta(\varepsilon)+\beta(\varepsilon'))}{\left[E_2-E_0-\varepsilon-\varepsilon'-2\Gamma_0\ln\frac{d}{|\varepsilon'+\varepsilon|}\right]}\ , \tag{40}$$

where $\Gamma_0=\tilde{\Gamma}/N$. This is similar to the single electron-hole-pair result of Evans and Gehring[8] except for the factor 2 multiplying the logarithm. The logarithm correction is naturally absorbed into E_2 which can be replaced by

$$E_2^*=E_2-2\Gamma_0\ln D/T^* , \tag{41}$$

while the f^1 energy E_1 is renormalized by the large-energy behavior at the integral in (40) to become E_1^*. Where

$$E_1^*=E_1-(N-1)\Gamma_0\ln D/T^* \tag{42}$$

and the energy scale T^* is so far undetermined. It is chosen in such a way that (40) and all physical qualities obtained from it be independent of E_1-E_2 and $\ln D$. Since the remaining integral on the right-hand side converges for $|D|>|E_1-E_2|$ we may write (40) in the form

$$\left[\tilde{E}-\varepsilon-(N-1)\Gamma_0\ln\frac{T^*}{(T^*+\tilde{E}-\varepsilon)}\right]\beta(\varepsilon)$$

$$=(N-1)\Gamma_0\int_{-\infty}^{0}d\varepsilon'\frac{\beta(\varepsilon')}{(T^*+E-\varepsilon-\varepsilon')} , \tag{43}$$

apart from $1/N$ sublogarithmic corrections. The singlet binding energy is given by $\tilde{E}=E_1^*-E$ while the charge-fluctuation energy scale T^* satisfies

$$T^*=E_2-E_1+(N-3)\Gamma_0\ln(D/T^*) , \tag{44}$$

which is the exact scaling-invariant quantity obtained by RDRN. Measuring the singlet binding energy relative to the f_2 state gives a similar scaling invariant, but with E_1 and E_2 reversed. The $O(1/N)$ calculation presented here therefore reproduces the perturbative scaling invariants found earlier.

In summary, we have formulated integral equations for the singlet quasiparticle energy of the f^1-f^2 Anderson model in a j-j-coupling scheme (in the limit of zero j-j coupling) to next-leading order in the $1/N$ expansion. For the low-energy properties we find that the specific heat, spin, and charge susceptibilities satisfy the same Fermi-liquid relation as in the f^0-f^1 Anderson model. As regards high-energy properties, the electron bandwidth and ionic energy difference can be eliminated in favor of charge-fluctuation energy scales which agree with results from perturbative scaling theory. The present formulation in terms of Goldstone diagrams can be simply extended to more realistic coupling schemes with the knowledge that both high- and low-energy properties are adequately described. Solution of the integral equations will yield static properties such as specific heat and spin susceptibility as a function of valence. Spectral properties can be calculated within this procedure and multiplet splittings should also be included. Such calculations should help determine whether impurity Anderson models or conventional band-theory descriptions are more appropriate for rare-earth systems other than cerium. A plethora of experimental data awaits such calculations.[20]

[1]K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975); H. R. Krishnamurthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1003 (1980); **21**, 1044 (1980).
[2]N. Andrei, K. Furuya, and J. H. Lowenstein, Rev. Mod. Phys. **55**, 331 (1983); A. M. Tsvelik and P. B. Wiegmann, Adv. Phys. **32**, 453 (1983); P. Schlottmann (unpublished).
[3]N. E. Bickers, Rev. Mod. Phys. **59**, 845 (1987).
[4]D. L. Cox, Phys. Rev. Lett. **59**, 1240 (1987).
[5]Y. Yafet, C. M. Varma, and B. A. Jones, Phys. Rev. B **32**, 360 (1985).
[6]N. Read, K. Dharmvir, J. W. Rasul, and D. M. Newns, J. Phys. C **19**, 1597 (1986).
[7]A. C. Nunes, J. W. Rasul, and G. Gehring, J. Phys. C **19**, 1017 (1986).
[8]S. M. M. Evans and G. Gehring, J. Phys. Condens. Matter **1**, 3095 (1989).
[9]T. Saso, J. Magn. Magn. Mater. **76-77**, 176 (1988); T. Pruschke, Physica B **163**, 553 (1990); H. Keiter and Q. Qin, *ibid.* **163**, 594 (1990) have extended the NCA to include finite U.
[10]Y. Shimizu, O. Sakai, and T. Kasuya, Physica B **163**, 401 (1990).
[11]F. C. Zhang and T. K. Lee, Phys. Rev. B **28**, 33 (1983); J. W. Rasul and A. C. Hewson, J. Phys. C **16**, L933 (1983); **17**, 2555 (1989); **17**, 3337 (1989).
[12]N. Read and D. M. Newns, Adv. Phys. **36**, 799 (1987).
[13]N. Read, Ph.D. thesis, University of London, 1985.
[14]J. W. Rasul (unpublished).
[15]A. Yoshimori, Prog. Theor. Phys. **55**, 67 (1976).
[16]P. Schlottmann, Phys. Lett. **100A**, 509 (1984).
[17]N. Grewe and H. Keiter, Phys. Rev. B **24**, 4420 (1981).
[18]J. H. Jefferson, J. Phys. C **10**, 3589 (1977).
[19]F. D. M. Haldane, Phys. Rev. Lett. **40**, 416 (1978).
[20]J. W. Allen, J. Magn. Magn. Mater. **76-77**, 324 (1988).