Solution of the Kondo Problem by Diagrammatic Methods

S. E. Barnes
Physics Department, University of Miami, Coral Gables, Florida 33124
(Received 27 December 1983)

A self-consistent parquet approximation is shown to give exact results for the Kondo problem in the scaling limit.

PACS numbers: 75.20.Hr

By concepts devised by Gell-Mann and Low,[1] Feynman-diagram methods have been used to derive scaling laws for the weak-coupling limit of the Kondo problem.[2] However, it seems to be widely believed[3,4] that such methods are incapable of dealing adequately with the crossover to strong coupling. After the numerical work of Wilson[4] (and recent Bethe-*Ansatz* calculations[5]) it is known that this crossover is characterized by the "magic" ratio $W' = (T_H/T_0) = (\pi/e)^{1/2}$, where the zero-temperature susceptibility is $\chi = \mu^2/\pi T_0$ and where T_H is the energy scale which enters, e.g., the formula $g = \frac{1}{2}[\ln(H/T_H)]^{-1}$ for the high-field coupling constant. Here H denotes the magnetic field. The acid test of any approach to the Kondo problem is its ability to reproduce this number.

In this Letter I wish to report the derivation, by diagram methods, of an analytical scaling law which is not only valid in the weak-coupling limit but which also spans the crossover to strong coupling. The results obtained here agree with those obtained via the aforementioned methods and, in particular, the magic crossover ratio $W' = (\pi/e)^{1/2}$ is rederived. To the author's knowledge this is the first realization of such a weak-to-strong analytic scaling theory.

The traditional view[3,4] has held that the effective coupling constant approached infinity as the energy scale is decreased. If this were to imply a divergent interaction vertex, all diagrams would be important to the crossover and the task would be impossible by the present methods. At least for the regularization(s) used here this is incorrect; the impurity self-energy $\Sigma \sim |\rho J|^{1/2} D \exp(1/\rho J)$ acts as a cutoff in the strong-coupling limit, i.e., the logarithmic integrals $I \sim \ln(\Sigma/D) \sim 1/\rho J$. The leading logarithmic terms are of order ρJ and other terms are small by factors of ρJ in the scaling limit, i.e., when $J \rightarrow 0$, $D \rightarrow \infty$ with T_K fixed. However, as will be seen, the results are in fact in total accord with the dictates of the Nozières[6]-Wilson fixed point.

The Hamiltonian is written as

$$H = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} - (J/N) \sum_{kk'\sigma\sigma'} a^\dagger_{k\sigma} (\mathbf{S}\cdot\mathbf{s} + \tfrac{1}{4})_{\sigma\sigma'} a_{k'\sigma'}. \tag{1}$$

Here $\mathbf{S}$ ($\mathbf{s}$) refers to the impurity (electronic) spin. The irrelevant potential-scattering term represented by the $\frac{1}{4}$ is added to simplify the diagram structure. All matrix elements are $+\frac{1}{2}$ and there are no longitudinal matrix elements for opposite spins. The g factors for the conduction electron and impurities are both taken equal to 2 ($g = 2$). The Abrikosov projection technique is used[7] and the temperature is 0.

The idea is to identify a suitable quantity which will be determined by a self-consistent equation. The value of the two-particle self-energy[8] Σ for the transverse susceptibility is chosen. This self-energy enters as a dressing in the relevant diagrams. The detailed justification of the methods, the particular sequence of diagrams to be summed, cancellations, etc., will necessarily have to appear elsewhere.[9] Here are presented scaling-theory arguments which represent the most transparent way to describe the results.

The calculation involves two distinct steps and even two different regularizations, i.e., ways of taking boundary conditions. The first step is to set up a self-consistent parquet-type approximation for $\Sigma(h)$, where $h = (1 + \frac{1}{2}\rho J) g \mu_B H$ is the Zeeman energy including the $O(J)$ term. Included are many vertex corrections. The result is a scaling equation which is solved to give the low-field, strong-coupling, scale $\Sigma(h=0) = 4\pi T_0$. The regularization used here is the standard one, i.e., $1/N \rightarrow 0$ before $s \rightarrow 0$, where s is the infinitesimal included in the frequency $(\omega_0 + is)$. This amounts to specification of outgoing waves as the boundary condition. The second step is the calculation of the conduction-electron scattering matrix. It is desired to obtain the quasiparticle energies directly. As is well known, exact eigenstates result if the order of the above limits is interchanged, i.e., $s \rightarrow 0$ then $1/N \rightarrow 0$. The associated boundary condition specifies standing waves. However, usually this causes the scattering matrix to become highly singular with singularities separated by $2D/N$, the separation between energy levels. Here, for states close to the Fermi energy ϵ_F, this problem does not arise. This can be anticipated from Nozières's discussion[6] of the ground state. The conduction electrons are excluded from the "central cell." This results in the phase shift $\pi/2$. The remaining scattering is weak and involves *inelastic* scattering via an excited (triplet) state of the impurity. Since the intermediate state involves the energy separation between the triplet and singlet there are no singularities until this energy is exceeded.

The conduction-electron scattering matrix is constructed with the same parquet-type approximation and the same scaling equation results; however, now reflecting the different boundary condition, physical quantities are related to the r matrix rather than the usual t matrix. As is well known, the former real quantity is *not* given by the imaginary part of the latter but rather new real solutions of the scaling equation are needed. The actual procedure followed illustrates the beauty of the scaling approach. Given first the energy scale $4\pi T_0$ obtained from the first part of the calculation and a second boundary condition (see below), the low-energy, small-field results follow by scaling from a small to a larger cutoff, i.e., the conventional scaling direction is reversed. Specifically, one scales from zero conduction-electron cutoff to some finite energy ϵ. A given diagram has, say, n renormalized vertices, each of order unity, and $n-1$ conduction-electron lines. However, each intermediate state contains the impurity self-energy $\sim 4\pi T_0$ and hence each conduction-electron integration introduces a small factor $\epsilon/4\pi T_0$, i.e., the diagram is of order $(\epsilon/4\pi T_0)^{n-1}$. This ability to perform systematic expansions about the strong fixed point is an important methodological advance which can be extended to the corresponding lattice problems. Given this series for the quasiparticle energies, the susceptibility, specific heat, and phase shift are easily calculated.

The present scaling formalism differs from that of Abrikosov and Migdal[2] because of a different choice of "invariant charge." It is this different choice which makes the problem tractable by diagrammatic methods.

The development can be related to the poor man's scaling technique; see Ref. 3. Consider the diagrams shown in Fig. 1. They are scaled with the magnetic field as the cutoff, i.e., the change $d\Sigma$ in the diagram is calculated as the field is reduced by dh. Taking such a derivative amounts to restricting the conduction-electron line which links the ends to lie in the interval $h/2 \rightarrow h/2 + dh/2$ or $-h/2 \rightarrow -h/2 - dh/2$. What is left is the effective conduction-electron–impurity interaction vertex denoted by g:

$$g = d\Sigma/dh, \tag{2}$$

A second derivative forces two lines to lie in these intervals and the result can be represented by a single bubble diagram with renormalized vertices at both ends as illustrated in Fig. 2. Because of the thermal factors $1-n_k$ and $n_{k'}$, k lies in the first and k' in the second interval. Thus with bare impurity lines one has

$$d^2\Sigma/dh^2 = 2g^2/h.$$

Here g is defined with a prefactor such that $g = \frac{1}{2}\rho J$ in the extreme weak-coupling limit. With Eq. (2) the scaling equation takes the familiar poor man's form:

$$dg/dh = 2g^2/h.$$

The principal innovation is to make this calculation self-consistent. Because of the two-particle nature of the calculation and the existence of vertex corrections, this step is complicated to execute. However, the result is simple:

$$d^2\Sigma/dh^2 = -2g^2/[\Sigma(h) - h],$$

or

$$(\Sigma - h)\, d^2\Sigma/dh^2 + (d\Sigma/dh)^2 = 0, \tag{3}$$

which is the new scaling equation and central result. It is a universal scaling law for Σ as a function of h. As defined, $\Sigma(h)$ is the value of the two-particle self-

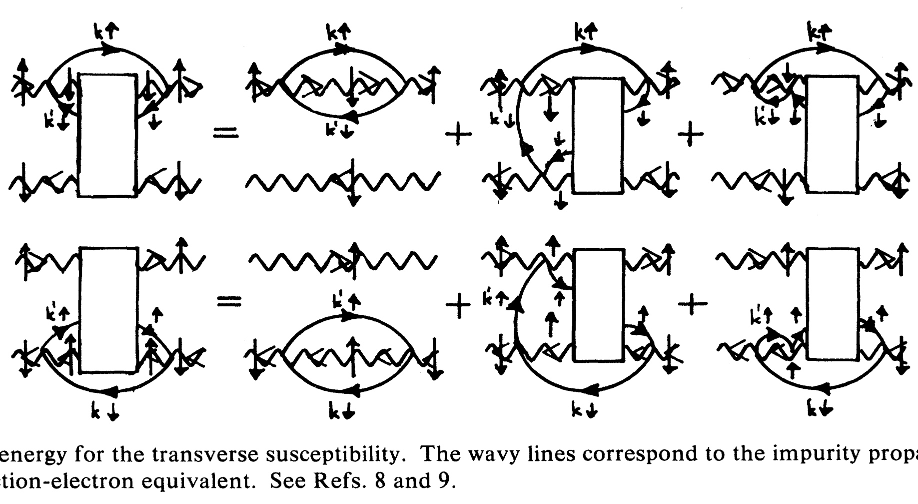

FIG. 1. The self-energy for the transverse susceptibility. The wavy lines correspond to the impurity propagators; the straight lines are the conduction-electron equivalent. See Refs. 8 and 9.

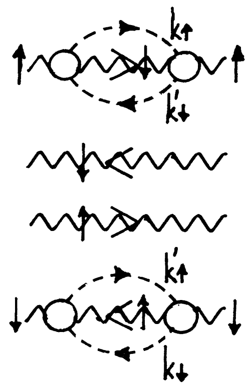

FIG. 2. The second-order scaling diagram. Dashed conduction-electron lines are restricted to the intervals of width dh and the large circles represent renormalized vertices.

energy *on energy shell.*

The sign of this quantity in the denominator of the right-hand side of the first line of (3) looks wrong. One might expect the relevant intermediate-state energy to be $h+\Sigma(h)$. This is not the case because with the relevant, i.e., zero-frequency, argument only the longitudinal self-energy contributes to this intermediate-state energy which acts as the cutoff. This is equal in magnitude to Σ except that it contains no $O(J)$ term and a careful accounting of these first-order terms is required. It is easily checked, with the modification $h \rightarrow (1+\frac{1}{2}\rho J)h$, that the next to leading $O(J^3)$ terms are correctly given. This scaling equation leads to an energy scale which contains the prefactor $|\rho J|^{1/2}$, indicating that it accounts correctly for the next to leading divergence in all orders [see Eq. (5b) below].

With the substitution $y=\ln[(\Sigma-h)/D]$, (3) can be written as

$$(dg/dy)=(1/2)g^2/(1-g), \tag{4}$$

which agrees with the usual approach[2] for $g \ll 1$.

Equation (4) is integrated and matched to the relevant asymptotic expansion

$$\rho J/(1+\tfrac{1}{2}\rho J)+(\rho J)^2[\ln(h/2D)+i\pi/2]+\ldots$$

for large h. The result is

$$(\tfrac{1}{2})[1/g+\ln g]+\ln[(\Sigma-h)/K]=0, \tag{5a}$$

where the integration constant (and energy scale) is

$$K=-2De^{1/2}|\rho J/2|^{1/2}\exp(1/\rho J). \tag{5b}$$

The factor $e^{1/2}$, part of W', appears because of the redefinition $h \rightarrow (1+\frac{1}{2}\rho J)h$ which was needed to account correctly for the $O(J)$ terms.

The result of integrating (5) is not very useful. Instead, the special properties of (3) are used. It is invariant to the transformation $\Sigma \rightarrow \Sigma+a$ and $h \rightarrow h+a$. The quantity a is equivalent to the second integration constant.

It should be noted that the asymptotic, $h \gg K$, solution for g is given directly by (5) by dropping Σ. It follows that the second integration constant a *cannot* be determined by matching solutions to such perturbative expansions.

A given a is equivalent to fixing the value of g for $h=0$. This value of g is determined by requiring $\Sigma(h)$ to reflect invariance to time reversal. First one notes that relaxation eventually involves the production of particle-hole pairs and a phase-space volume which is proportional to h. It must be that $\mathrm{Im}\{\Sigma\}=0$ for the long-time limit, $h=0$, i.e., Σ is real. If Σ is to reflect time-reversal symmetry the real part must be of the form $a+bh^2$, i.e., $\{\mathrm{Re}\,d\Sigma/dh\}=0$ for $h=0$. This gives $g=2i/\pi$ for $h=0$ and

$$\Sigma=4\pi T_0=(e\pi)^{1/2}D|\rho J|^{1/2}\exp\{1/|\rho J|\}. \tag{6}$$

The second $\pi^{1/2}$ component of W'/π appears with this step.

The nature of the conduction-electron states near the Fermi surface are a little unusual. The physics which emerges from the analysis[9] has the following features: (i) The impurity ground state is a singlet, $|S\rangle$, with the gap $4\pi T_0$ separating it from the triplet states, $|T\rangle$ (see below). (ii) As discussed in the second paragraph after (1), there is an effective conservation principle which implies, in the strong limit, that there is only mixing of conduction-electron states which lie close to the Fermi surface with ones outside a region of width $4\pi T_0$ about the Fermi surface.

The "self-energy," or energy shift, associated with the quasiparticle states is calculated by evaluating the poles of the scattering (r) matrix. As would be expected, the effective vertices are again given by $g=d\Sigma/dh$, where Σ obeys the scaling equation (4). However, for the reasons already stated, the required solutions are real and different from that obtained above. The $J\mathbf{S}\cdot\mathbf{s}$ interaction only has matrix elements which connect the singlet $|S\rangle$ to the triplet $|T\rangle$. There remains a multitude of processes. A scattering process which involves the states $|S\rangle$ to $|T\rangle$ and back to $|S\rangle$ has an associated minimum intermediate-state energy $4\pi T_0$, i.e., the separation between $|S\rangle$ and $|T\rangle$. The corresponding contribution is clearly not singular on the small scale $2D/N$. However, the process $|S\rangle$, $|T\rangle$, $|S\rangle$, $|T\rangle$, and $|S\rangle$ *would* involve, in the middle $|S\rangle$ state, energies within $\sim 2D/N$ of the ground state and *is* singular on this scale. However, such contributions are negligible since one finds[9] that the integration corresponding to the $|T\rangle$ state, first, involves a minimum energy difference of $4\pi T_0$ and, second, by particle-hole symmetry, is symmetric relative to the Fermi energy. Such integrals involve only band-edge effects and introduce factors of ϵ/D for each $|T\rangle$ intermediate state. Here ϵ denotes the quasiparticle energy of interest. It is found,[9] in the strong-coupling limit, that one needs account only for processes which correspond to a contribution proportional to g. Thus, for a *fixed total spin* a typical result for the quasiparticle "self-energy," in the strong limit, is

$$\sigma_\sigma(\epsilon_{k\sigma}) = (1/2\rho N) g(\epsilon_{k\sigma} - \sigma h). \quad (7)$$

There are, in fact, two branches for the vertex function, i.e., g^* associated with spin-up and g with spin-down electrons with energies $\epsilon_{k\sigma} < \epsilon_p$. This is easy to see from simple considerations: The finite value of Σ for $h=0$ has an immediate and very strong consequence. Directly, the double degeneracy of the impurity in the absence of interactions, in zero field, is lifted. This leaves the ground state *of the impurity* nondegenerate. If it is to satisfy time-reversal symmetry, this state must also be a spin singlet. (For the ferromagnetic problem Σ is zero for $h=0$ and the moment is not compensated. The $S > \frac{1}{2}$ problem can be understood in a similar way.)

The compensation of the impurity is then reflected by strong restrictions on g and g^*. From Eq. (7), the phase shifts of the up and down quasiparticles are proportional to the effective vertices, i.e., $\delta_\uparrow/\pi = g^*/2$ and $\delta_\downarrow/\pi = g/2$. The problem reduces to a spin-dependent scattering problem and Friedel's sum rule can be applied to each scattering channel.

The ground state is arrived at by decreasing the field h from a large value such that in the weak limit the impurity spin is fixed in a near eigenstate $|S_z\rangle$. Since the impurity is neutral the net phase shift must be zero. This is reflected by a condition $g + g^* = 0$, i.e., the phase shifts for the two spin channels are equal but opposite. The relevant value of g is then dictated by Friedel's sum rule and the absence of a moment, i.e.,

$$g = -1 = -g^*. \quad (8)$$

The same result is obtained by time-reversal requirements in the full report of this work.[9]

For $h=0$, Σ is real and given by (6). It corresponds to the energy separation between the impurity states $|S\rangle$ and $|T\rangle$. Given that this is a physically significant energy, it must be independent of the regularization. Then (3), (6), (7), and (8) give the desired expansion about the strong-coupling fixed point:

$$\epsilon_{k\uparrow} = \epsilon^0_{k\uparrow} + (1/2\rho N)(1 - \epsilon_{k\downarrow}/2\pi T_0 + \ldots). \quad (9)$$

Here the equivalence of the phase shifts $\pm\pi/2$ has been used. This expression is of the same form as is given by Nozières's model[6]; it corresponds to a phase shift $\delta_0 = \pi/2$, i.e., the unitarity limit, a susceptibility $\chi = \mu_B^2/\pi T_0$, and a specific heat such that $R = [(\Delta\chi/\chi)/(\Delta C_v/C_v)] = 2$.

In order to calculate the crossover ratio, W', it is necessary to evaluate the high-field scale energy. The relevant quantity is the effective exchange $g = (\frac{1}{2}) \times \ln(H/T_H)$ in a large field, *ignoring band-edge effects.* The result, using $h = 2H$,[5] is

$$T_H = |\rho J|^{1/2}(D/4)\exp(1/\rho J). \quad (10)$$

The present method therefore reproduces Wilson's result for the crossover ratio $W' = (T_H/T_0) = (\pi/e)^{1/2}$ or, with the known result[5] for (T_H/T_K), his result for $(\pi T_0/T_K)$.

This work is supported in part by the National Science Foundation Solid State Theory Grant No. DMR 81-20827.

[1]M. Gell-Mann and F. Low, Phys. Rev. **95**, 1300 (1954).

[2]A. A. Abrikosov and A. A. Migdal, J. Low Temp. Phys. **3**, 519 (1970); M. Fowler and A. Zawadowski, Solid State Commun. **9**, 471 (1970).

[3]P. W. Anderson, Comments Solid State Phys. **5**, 73 (1973).

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

[5]See reviews by A. M. Tsvelick and P. B. Wiegman, Adv. Phys. **32**, 453 (1983), and N. Andrei, K. Furuya, and J. H. Lowenstein, Rev. Mod. Phys. **55**, 331 (1983).

[6]P. Nozières, J. Low Temp. Phys. **17**, 31 (1974).

[7]A. A. Abrikosov, Physics (Long Island City, N.Y.) **2**, 5 (1965).

[8]S. E. Barnes and J. Zitkova-Wilcox, Phys. Rev. B **7**, 2163 (1973); S. E. Barnes, J. Phys. F **7**, 2637 (1977).

[9]S. E. Barnes, to be published.