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Alternative renormalisation in the Kondo problem

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Abstract. Whereas the standard expansion of the 'quantum field theory' belonging to the s–d exchange Kondo Hamiltonian for a spin impurity in a paramagnetic host metal describes the high-energy scattering, the alternative renormalised perturbation expansion describes the low-energy scattering. In the high-energy regime the scattering centre acts as if it was an anti-ferromagnetically coupled spin, but in the low-energy regime it acts as if it was a spin of a different magnitude that is ferromagnetically coupled. Correspondingly, it is shown that two different Hamiltonians can give rise to the same field theory. In solid state physics this equivalence is the generalisation of the Schrieffer–Wolff transformation between the Anderson (or Wolff) model and the spin-$\frac{1}{2}$ Kondo Hamiltonian.

1. Introduction

Many of the properties of a Kondo system follow from the fact that a Kondo Hamiltonian gives rise to a renormalisable quantum field theory (Abrikosov and Migdal 1970, Fowler and Zawadowski 1971), where the 'field theory' is the large cut-off (Λ, the 'effective band width') asymptotic part of the theory given directly by the Hamiltonian. Here we study an alternative way of rearranging the perturbation series in order to extract this asymptotic part.

The Kondo Hamiltonian (for a review of early work see Kondo (1969)) studied herein has a single impurity-spin scattering centre interacting with a single scattering channel of conduction electrons. Cragg and Lloyd (1979a) have shown that all such rotationally invariant Hamiltonians can be mapped onto the canonical form

$$H = -J\int \mathrm{d}k \int \mathrm{d}k'\, c_k^\dagger \boldsymbol{S}_e c_{k'} \cdot \boldsymbol{S} + \int k c_k^\dagger c_k \,\mathrm{d}k \qquad |k| \leqslant \Lambda \tag{1.1}$$

where $\boldsymbol{S}_e$ is the spin-$\frac{1}{2}$ matrix belonging to the electron's spin and $\boldsymbol{S}$ is the spin operator belonging to the impurity spin. The fermi level is at zero, and the units are such as to make the fermi velocity unity. This makes the exchange constant J dimensionless, as befits a renormalisable theory. In real materials J is anti-ferromagnetic ($J<0$). It is also small, and so the standard expansions have been in powers of $-J\boldsymbol{S}_e \cdot \boldsymbol{S}$. However, the non-perturbative theories of Anderson *et al* (1970) suggest that the effective value of the exchange constant scales to a large value when the energies of interest become small (see also Anderson 1970, Nozieres 1975, 1978), and this has been confirmed by the numerical calculations of Wilson (1974, 1975). The expansion in this paper 'pretends' that J is large, and so it directly diagonalises the $-J\boldsymbol{S}_e \cdot \boldsymbol{S}$ term as part of the unperturbed system and then expands in powers of the transfer to and from the scattering site. Before renormalisation theory is applied, this is essentially an expansion

in powers of $1/J$. However, after the renormalisation of the theory it becomes the low-energy expansion of the original problem, as is suggested by the scaling arguments.

In this problem the simplest approach to renormalisation theory is that due to Ward (1951a, b). In this approach the basic step is to differentiate each completely resummed vertex function (amputated and irreducible) until its dimensionality, expressed in the form Λ^D, has D negative. Once this is done, the diagrammatic expansion may be reordered so that wherever an internal vertex combination belonging to $D \geqslant 0$ occurs, it occurs only as the completely resummed vertex function. In this rearranged series the only remaining explicit Λ-dependence is in the limits of integration over the momentum in electron lines joining such complete vertex functions; but these integrations can be extended to infinity, with errors only of the order of Λ^D that do not contribute to the asymptotic part as $D<0$. For vertex functions with $D \geqslant 0$, the above-differentiated series form the kernels of determining integral equations, and so all the Λ dependence is now contained in the integration constants of these integral equations. In the Kondo problem $D = 1 - E/2$, where E is the number of external electron lines belonging to the vertex function being considered. Consequently, the impurity self-energy, which is $D = 1$, gives rise to two renormalisation constants while the $D = 0$ T-matrix scattering vertex gives rise to one renormalisation constant.

The field theory was extracted from the given Hamiltonian theory in that step where the upper limit on the specified momentum integrations was extended to infinity. If ω is any external energy variable, then the above procedure has the effect of retaining all the functional dependence on ω/E_K, where E_K is the Kondo energy

$$E_K = (\text{constant})\Lambda(|J|)^{1/2}\, e^{1/J+O(J)}, \tag{1.2}$$

while at the same time eliminating any other ω/Λ-dependence. In the alternative expansion, the cut-off Λ appears explicitly in the unperturbed part of the Hamiltonian and the procedure is then not so clear-cut. On dropping some ω/Λ terms, one cannot be absolutely certain that they are not part of some subtle expansion of ω/E_K. However, when the ground-state spin is non-zero, each term in the perturbation expansion is a mixture of $\ln(\omega/\Lambda)^r$ with $r \geqslant 0$ and $(\omega/\Lambda)^s$ with $s > 0$ parts, as in the standard expansion, and the assumption is made that only the obviously larger first set of these need be retained. This leads to a set of Ward integral equations that possess the same number of renormalisation constants as before. Consequently, it again leads to a renormalisation-group equation that expresses the arbitrariness of the renormalisation point, and this in turn implies that all vertex functions are actually functions of ω/E_K, although it requires another assumption to say that this is the same Kondo energy as before. It also leads to the same Nozieres–Wilson Ward identities as hold for the standard expansion.

The existence of the renormalised alternative expansion also implies that two different Hamiltonians can both belong to the same field theory. In particular, a Hamiltonian with a small anti-ferromagnetic exchange constant and an impurity-spin S can be made equivalent to a large ferromagnetic exchange constant Hamiltonian with spin $S' = S - \frac{1}{2}$. To help validate the theory some Wilson-style numerical calculations have been made, and these seem to confirm that these two quite different Hamiltonians both give rise to identical many-particle eigenvalues when the exchange constants are correctly related.

Even in the limit $S' \to 0$, a ferromagnetic spin-S' Hamiltonian can be mapped onto an anti-ferromagnetic spin-$\frac{1}{2}$ impurity. This limiting case is actually equivalent to the symmetric Anderson (1961) or Wolff (1961) Hamiltonian for an impurity that induces a strong electron–electron interaction locally at the impurity site. In this case, the

equivalent Hamiltonian theory is the generalisation to arbitrary order in perturbation theory of the Schrieffer–Wolff (1966) transformation between the Anderson Hamiltonian and the s–d exchange Kondo Hamiltonian.

In real materials the number of scattering channels and the magnitude of the spin are related so as to produce a zero-spin ground state (see Cragg *et al* 1980, Blandin and Nozieres 1980) but, despite its interest, this paper does not discuss the low-energy expansion of the anti-ferromagnetic spin-$\frac{1}{2}$ impurity. When the ground-state spin is zero, the basic renormalised vertex of this paper (see equation (3.9) below) is identically zero, and the terms in the perturbation series expansion no longer clearly divide into large and small parts. It would appear that if the strategy underlying this paper is to be used to produce this low-energy expansion, then the basic renormalised vertex will have to be a four-electron line vertex (such as occurs as a bare Hamiltonian term in the Anderson model) and not the two-electron line T-matrix vertex of this paper.

2. The alternative expansion

If J was large then the central interaction site, and not the conduction electron states, would be diagonalised first.

The local orbital creation operator belonging to (1.1) is

$$f^{\dagger} = \frac{1}{(2\Lambda)^{1/2}} \int c_k^{\dagger} \, \mathrm{d}k. \tag{2.1}$$

In terms of this operator the first term in (1.1) is

$$H_{\mathrm{I}} = -2\Lambda J f^{\dagger} \boldsymbol{S}_{\mathrm{e}} f . \boldsymbol{S} \tag{2.2}$$

and this is the term which is to be diagonalised first. Note that this term now explicitly involves the cut-off Λ.

The zero-electron state and the two-electron state are eigenstates of H_{I} with spin S and zero eigenvalue. The one-electron states have a spin of either $S' = S + \frac{1}{2}$, or $S' = S - \frac{1}{2}$, and belong to the eigenvalues

$$E_{\pm} = -\Lambda J[-\tfrac{1}{2} \pm (S + \tfrac{1}{2})]. \tag{2.3}$$

The specific form of these one-electron states is

$$|S \pm \tfrac{1}{2}, M\rangle = \sum_{\sigma} \mathrm{sgn}(-\sigma) f_{-\sigma}^{\dagger} |S, M + \sigma\rangle C_{\sigma}^{\pm}(M) \tag{2.4}$$

where the Clebsch–Gordan coefficients are given by

$$C_{\sigma}^{\pm}(M) = \{\mathrm{sgn}(\sigma) \text{ if } + \text{ else } 1 \text{ if } -\} \left(\tfrac{1}{2} \mp \mathrm{sgn}(\sigma) \frac{M}{2S+1} \right)^{1/2}. \tag{2.5}$$

The orthogonal scattering states associated with the local state (2.1) have a phase shift of $\pi/2$ with respect to the states created by $c_k^{\dagger}$, and are given by

$$q_k^{\dagger} = c_k^{\dagger} + \int \mathrm{d}k' \, c_{k'}^{\dagger} \frac{1}{k^{+} - k'} \left(-\frac{1}{G_0(k^{+})} \right) \tag{2.6}$$

where $G_0(k^+)$ is the local-state-to-local-state Green function

$$G_0(k^+) = \int \mathrm{d}k' \frac{1}{k^+ - k'} = \ln\left|\frac{\Lambda + k}{\Lambda - k}\right| - \mathrm{i}\pi. \tag{2.7}$$

The notation 'k^+' means that the imaginary part of the symbol is positive, and here infinitesimal.

In terms of these states the Hamiltonian (1.1) is (cf Lloyd and Osborne 1971)

$$H = H_\mathrm{I} + \frac{(2\Lambda)^{1/2}}{\pi} \int \mathrm{d}k\ (\Gamma(k) q_k^\dagger f + \mathrm{HC}) + \int k q_k^\dagger q_k\, \mathrm{d}k \tag{2.8}$$

where

$$\Gamma(k) = \pi / G(k^-), \tag{2.9}$$

so that

$$|\Gamma(0)|^2 = 1. \tag{2.10}$$

The required time-ordered expansion of the total Green function is obtained by expanding the resolvant operator $1/(\omega^+ - H)$ in powers of the second term in (2.8). Feynman rules make the discussion of renormalisation theory much easier, and these can be derived from the time-ordered rules by decomposing the total propagator for the total system as a function of the total energy parameter into the individual particle propagators, each with their own individual energy parameters, by means of formulae like

$$\mathrm{i}(\omega^+ - \epsilon_1 - \epsilon_2)^{-1} = \int \frac{\mathrm{d}\omega_1}{2\pi} \int \mathrm{d}\omega_2\, \delta(\omega - \omega_1 - \omega_2) \mathrm{i}(\omega_1^+ - \epsilon_1)^{-1} \mathrm{i}(\omega_2^+ - \epsilon_2)^{-1}. \tag{2.11}$$

Starting from the time-ordered expansion bypasses the fact that Wick's theorem is not applicable to spin operators.

In diagrammatic form the time-ordered rules are as follows.

(i) A single impurity line always exists, and its excitation states are represented by

(2.12)

Here M is the z component of total spin; (a) represents the single-electron state with total spin $S' = S \pm \frac{1}{2}$, (b) represents the two-electron state and (c) represents the zero-electron impurity state.

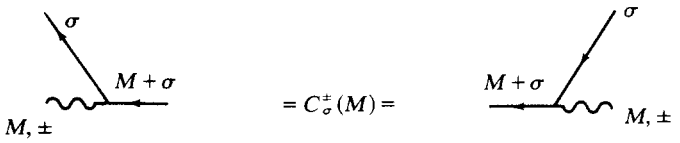
(ii) Conduction electron excitations from the fermi sea are represented by

(2.13)

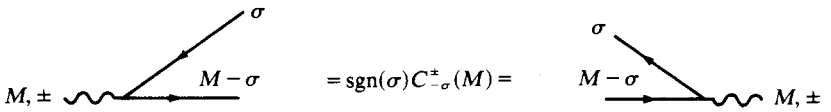
Here σ is the spin component of the electron, (a) is a particle excitation with $0 \leqslant k \leqslant \Lambda$ and (b) is a hole excitation with $-\Lambda \leqslant k < 0$.

(iii) The lines join at vertices as in (2.14), in such a way that the single impurity line is continuous, as are also the directed electron lines. The z component of spin is conserved at each vertex, but not the electron momentum. Each vertex gives a factor $[(2\Lambda)^{1/2}/\pi]\Gamma(k)$ where an electron leaves, the complex conjugate of this where it

arrives, and the Clebsch–Gordan factors



(2.14*a*)

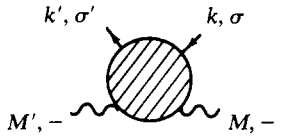


(2.14*b*)

(iv) There is a -1 fermion factor for each electron line 'loop', and a -1 factor for each hole line, with (2.12*c*) also counted as a hole line. Each free propagation region gives $(\omega^+ -$ impurity energy + hole line energies − particle line energies$)^{-1}$. The internal spin labels are summed over, and the internal momentum labels are integrated over.

The Feynman rules are the straightforward analogue of these and will not be explicitly listed.

The physical T-matrix scattering vertex is then the complete sum of diagrams like



(2.15)

divided by the non-interacting propagators associated with the external legs (i.e. amputated), multiplied by a $Z^{1/2}$ factor for each external impurity leg where $Z^{1/2}$ is the overlap between the true ground-state wavefunction and the bare impurity state as implied by (2.15), and with the impurity energy put equal to the true ground-state energy.

Consider the scattering contribution of the two diagrams

(2.16)

when the external electrons have zero energy and J is negative. The ground state of the impurity is then of spin $S' = S - \frac{1}{2}$ and has energy E_- as given by equation (2.3). Rule (iv) gives the energy denominator here as just $1/\omega^+$ but, as the discussion of the T-matrix shows, this energy should be of the order of E_-, and so we shall measure the energy parameter from the ground-state energy and take the energy denominator as being $1/(\omega^+ + E_-)$. The Clebsch–Gordan coefficients of (2.14) combine as

$$C^-_{\sigma'}(M')C^-_{\sigma}(M) \equiv \tfrac{1}{2}\delta_{M'M}\delta_{\sigma'\sigma} + \frac{2}{2S+1}[\boldsymbol{S}_e]_{\sigma'\sigma}\cdot[\boldsymbol{S}']_{M'M} \tag{2.17a}$$

$$\operatorname{sgn}(\sigma)C^-_{-\sigma}(M')\operatorname{sgn}(\sigma')C^-_{-\sigma'}(M) \equiv \tfrac{1}{2}\delta_{M'M}\delta_{\sigma'\sigma} - \frac{2}{2S+1}[\boldsymbol{S}_e]_{\sigma'\sigma}\cdot[\boldsymbol{S}']_{M'M} \tag{2.17b}$$

to produce the matrix elements $[S']_{M'M}$ of a spin-$S' = S - \frac{1}{2}$ operator. When the -1

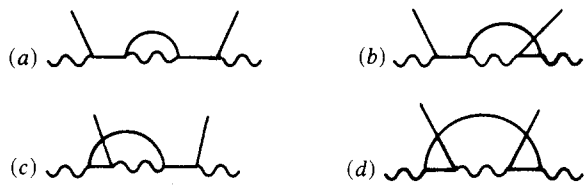
fermion factor of diagram (b) is included, the net interaction has the form

$$-K\boldsymbol{S}_e \cdot \boldsymbol{S}' \tag{2.18}$$

with

$$K = -\frac{8}{\pi^2(2S+1)} \frac{\Lambda}{\omega^+ + \Lambda J(S+1)}. \tag{2.19}$$

The standard expansion describes a series of interactions between the original anti-ferromagnetic spin-S impurity and the conduction electrons, but this large-J expansion describes the interactions of an effective ferromagnetic spin-$S' = S - \frac{1}{2}$ scattering centre. The logarithmic divergences first appear in perturbation theory at second order in the spin interaction, and so here they first appear in the diagrams



(2.20)

3. The alternative form for the renormalised field theory

The above expansion is very similar to the standard expansion of a Hamiltonian with the interaction term $-K\boldsymbol{S}_e \cdot \boldsymbol{S}'$, but it is not identical to it as vertex functions like (2.19) are energy dependent and only the large-Λ asymptotic part

$$K = -\frac{8}{\pi^2(2S+1)} \frac{1}{J(S+1)} \tag{3.1}$$

is energy independent like a true Hamiltonian term. But it is not valid just to take the asymptotic part of terms like (2.19) and then to treat the result as a Hamiltonian term. For example, the denominator $\Lambda/(\omega^+ + \Lambda J(S+1) - k)$ occurs in diagram (2.20b). The equivalent of (3.1) would be just to replace this by $1/J(S+1)$, but evaluating the diagram with this expression replacing the true one leads to an incorrect asymptotic value for the total diagram, as $k \sim \Lambda$ during the integration. In this section the formal field-theory method of extracting the correct asymptotic part is discussed.

In the Ward approach the diagrams for a vertex function with $D \geq 0$ are differentiated with respect to external energy variables. These differentiations are performed propagator by propagator, and then the diagrams are resummed using the differentiated propagators as reference points. Fortunately, the differentials of non-ground-state impurity lines give only Λ^{-1} contributions to these negative-D forms (cf the effect of differentiating (2.19)). The same is true for differentials of a ground-state impurity line itself, when it occurs as part of a self-energy term belonging to an excited impurity line. This means that when the series is reordered about the differentiated propagator so as to make each vertex a complete T-matrix vertex function, the only T-matrix required is that T-matrix in which a single electron is scattered off the impurity in its ground state, with the impurity returning to its ground state after the scattering is complete.

By 'T-matrix' we always mean that vertex function which has two external electron lines, $E = 2$. Also present are $E \geq 4$ vertex forms that cannot be decomposed into such

$E = 2$ T-matrices. In the asymptotic limit these do not contribute to the Ward kernels either. With $E \geqslant 4$, such terms are of order Λ^{-1} or less, and in a negative-D kernel these cannot combine into any larger-order contribution. They can, though, give finite contributions to the inhomogeneous terms of the Ward integral equations.

The self energy for the ground-state impurity propagator has $D = 1$, and so it is differentiated twice to get $\Sigma''(\omega)$ which has $D = -1$. The expression for the self energy itself therefore contains two integration, or renormalisation, constants. These are given by the relation

$$(\omega - \Sigma(\omega))^{-1} = Z^{1/2}(\omega_R)(\omega - M(\omega_R) - \Sigma_R(\omega; \omega_R))^{-1} Z^{1/2}(\omega_R) \tag{3.2}$$

where ω_R is arbitrary,

$$\Sigma_R(\omega; \omega_R) = \int_{\omega_R}^{\omega} d\omega_1 \int_{\omega_R}^{\omega_1} d\omega_2 \, Z^{1/2} \Sigma''(\omega_2) Z^{1/2} \tag{3.3}$$

and the two renormalisation constants are the wavefunction renormalisation constant

$$Z(\omega_R) = 1/(1 - \Sigma'(\omega_R)) \tag{3.4}$$

and the renormalised mass constant

$$M(\omega_R) = Z^{1/2}(\Sigma(\omega_R) - \omega_R \Sigma'(\omega_R)) Z^{1/2}. \tag{3.5}$$

In this problem the renormalised mass is actually a 'binding energy'. In the standard expansion it can be removed by changing all impurity energy variables according to

$$\omega' = \omega - M(\omega_R). \tag{3.6}$$

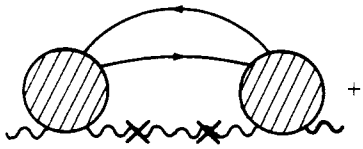
In the present expansion a similar change has to be made, not now for convenience but in order to put the correct Λ-dependence into the non-ground-state denominators, as in the example at the end of § 2. These Λ-factors are to be cancelled against those in the numerators when the asymptotic limit is taken. This limit is independent of the arbitrary renormalisation point ω_R', as

$$\partial M(\omega_R')/\partial \omega_R' = -\omega_R' Z \Sigma''(\omega_R)/(1 + \omega_R' Z \Sigma''(\omega_R)), \tag{3.7}$$

and it is shown below that $Z\Sigma''(\omega_R)$ is of order unity. Hereafter we suppress the primes on these variables.

The renormalisation constant $Z^{1/2}(\omega_R)$ will always be combined with an abutting vertex. Hence it, also, does not appear explicitly in the formalism.

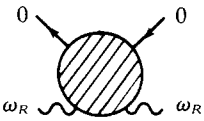
It is the integrand in (3.3) that is the $D = -1$ quantity and that is given a diagrammatic expansion in which each vertex is a complete T-matrix:

$Z^{1/2}\Sigma''(\omega)Z^{1/2} =$  $+ \ldots .$ (3.8)

Here the crosses denote differentiations of the renormalised ground-state impurity propagator (the middle term in (3.2)), and so the momentum integrations over the electron lines can be extended to infinity. Any explicit $\Gamma(k)$ factor associated with these lines only contributes its $k = 0$ value (see equation (3.9) below), and so the momentum integrations do not contribute any Λ-dependence to the final result. With the renormalised mass constant M now buried inside the vertex, and with the wavefunction

renormalisation constant Z also absorbed into the vertices, there is no explicit Λ-dependence in the series (3.8).

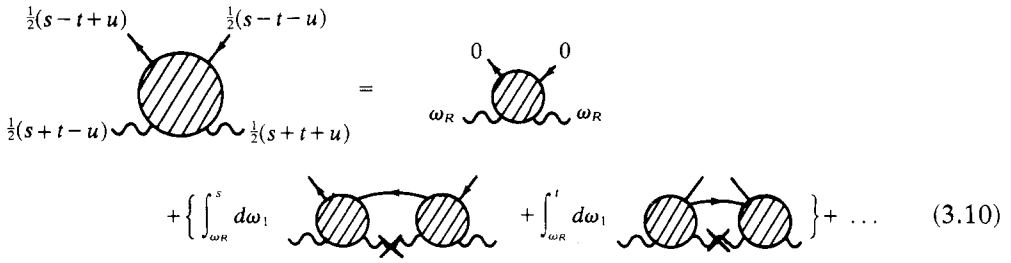
Arguments like these show that any physical vertex function can be determined once the complete T-matrix vertex function is known, without introducing any new explicit Λ-dependence. The same argument also shows that the T-matrix vertex function itself can be similarly determined once its value is known for any given set of external energies. We take the renormalisation point as in



$$\equiv -K_R(\omega_R)\boldsymbol{S}_e \cdot \boldsymbol{S}' \tag{3.9}$$

where ω_R is fixed but arbitrary (although negative for simpler analytic properties). The entire field theory is then specified once the renormalised exchange constant $K_R(\omega_R)$ is given, and all the cut-off dependence of the theory is contained in this constant.

To second order the Ward integral equation for the T-matrix is



(3.10)

When solved by successive substitutions, the differentiated denominator is $-1/(\omega_1^+ - k)^2$, which integrates as

$$\int_0^\infty -\frac{\mathrm{d}k}{(\omega_1^+ - k)^2} = \frac{1}{\omega_1^+}. \tag{3.11}$$

Substituting, and taking the integrals over ω_1, gives

$$T(s,t,u) = \{(-K_R) - \tfrac{1}{2}(-K_R)^2[\ln(-s^+/-\omega_R) + \ln(-t^+/-\omega_R)] + \ldots\}\boldsymbol{S}_e \cdot \boldsymbol{S}' + \tfrac{1}{4}S'(S'+1)(-K_R)^2 \ln(-s^+/-t^+) + \ldots. \tag{3.12}$$

This is the same as the standard expansion, excepting that J_R has become replaced by K_R, and $\boldsymbol{S}$ has been replaced by $\boldsymbol{S}'$.

The original $1/J$ expansion now re-emerges in the asymptotic expansion of the inhomogeneous term in (3.10),

$$K_R(\omega_R) = \left(\frac{-8}{\pi^2(2S+1)}\frac{1}{J(S+1)}\right) + \left(\frac{-8}{\pi^2(2S+1)}\frac{1}{J(S+1)}\right)^2\left[\ln\left(-\frac{\omega_R}{\Lambda}\right) + C_2\right] + O\left(\frac{1}{J^3}\right) \tag{3.13}$$

where, using the method in Cragg and Lloyd (1979a),

$$C_2 = \int_0^\infty \ln\left(\frac{k}{\Lambda}\right)\frac{\partial}{\partial k}|\Gamma(k)|^2\,\mathrm{d}k = \int_0^1 \mathrm{d}x \ln x \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\pi^2}{\pi^2 + \ln^2|(1+x)/(1-x)|}\right) = \frac{\pi^2}{2}. \tag{3.14}$$

4. The alternative expansion is actually a low-energy expansion

The renormalised exchange constant is actually a function of ω/E_K. The validity of the expansion then depends on the ratio of the energies involved to the Kondo energy rather than on the magnitude of J.

Section 3 implies that if the renormalisation point is altered, then

$$\omega_R \frac{d}{d\omega_R} K_R(\omega_R) = \psi(K_R) \tag{4.1}$$

with the right-hand side being a function of K_R only. Explicitly (Abrikosov and Migdal 1970),

$$\psi(K_R) = K_R^2 + \tfrac{1}{2}K_R^3 + \ldots \tag{4.2}$$

with the fourth-order term being the first to depend on the spin magnitude. This renormalisation-group equation is the generator of a substitution group, and so it can be integrated by putting

$$\frac{d}{dK_R}\Phi(K_R) = \frac{1}{\psi(K_R)} \tag{4.3}$$

to give

$$\Phi(K_R) = \ln(-\omega_R/E_K) \tag{4.4}$$

where

$$E_K = \Lambda \exp\{-\Phi[K_R(-\Lambda)]\}. \tag{4.5}$$

The small-J form of this Kondo energy is given by equation (1.2). This implies that K_R is a function of ω_R/E_K and not of any other combination of J and Λ.

In terms of the Kondo energy, (3.13) takes on the rather different looking form

$$K_R(\omega_R) = -1/\ln(-\omega_R/E_K) + \ldots \tag{4.6a}$$

which is similar to the standard expansion form

$$J_R(\omega_R) = -1/\ln(-\omega_R/E_K) + \ldots \tag{4.6b}$$

although the series are not identical in later terms as $S' \neq S$. The renormalised expansions are in powers of these renormalised exchange constants, and so the condition for the usefulness of either expansion is that the corresponding constant should be small. Note that the constant for the ferromagnetic expansion, K_R, is positive if $(-\omega_R) < E_K$, and that the constant for the anti-ferromagnetic expansion, J_R, is negative if $(-\omega_R) > E_K$.

In practice, the arbitrary renormalisation point ω_R is not totally arbitrary. The expansions of the vertex functions, such as expansion (3.12), contain logarithmic coefficients and these are made as small as possible if $|\omega_R|$ is made to be of the order of the external energies. Hence the renormalised exchange constants (4.6) are effectively small if all energies of interest are much larger than the Kondo energy, or if all energies of interest are much smaller than the Kondo energy. Numerical calculations (cf Cragg and Lloyd 1979b) show that it is the anti-ferromagnetic expansion in powers of (4.6*b*) that describes the high-energy regime, and that it is the ferromagnetic expansion in

powers of (4.6*a*) that describes the low-energy regime. Cragg (1980, Monash University thesis) has shown, in some detail, that the numerically calculated low-energy results are well fitted by expressions similar to these.

The solution given here does not fully determine the low-energy properties. There is an arbitrary integration constant in the equation defining the Kondo energy (4.3). If the large-J form of E_K is used in the low-energy expansions, then this does not matter, but in practice one wishes to use the small-J form of E_K in these equations. There is then still one undetermined multiplicative constant in the theory, as has been written into equation (1.2). Once this constant is known, say by a numerical calculation, the theory then fully determines the low-energy regime of the problem.

Nozieres (1974, 1975, 1978) has shown that to lowest order the temperature-dependent properties can be understood from a phenomenological Landau fermi liquid theory. *A priori* this theory contains two unknown constants, but these can be reduced to only one unknown constant by means of the Nozieres–Wilson relation. The remaining unknown constant is the analogue of the integration constant above.

The Nozieres–Wilson relation is actually a Ward identity. The proof given in Lloyd and Cragg (1979) is easily generalised to the present case of a non-zero ground-state spin, but a much easier proof may be given within the current formalism as it is already valid near the ground state. We shall sketch this proof as it helps validate the way in which the asymptotic part has been taken.

Consider an arbitrary vertex function evaluated with each of its external electron line energies, typically ω_e, changed by a constant μ, the same for each line, to $\omega_e - \mu$, while its external impurity line energies are unaltered. Here μ is finite, but small compared with Λ so that μ/Λ is zero as far as the asymptotic part is concerned. Under the Feynman rules, this change in the external energies is equivalent to changing all the internal electron propagators, including those in 'closed loops', from

$$\mathrm{i}/(\omega - k \pm \mathrm{i}0\ \mathrm{sgn}(k)) \qquad \text{to} \qquad \mathrm{i}/(\omega - \mu - k \pm \mathrm{i}0\ \mathrm{sgn}(k)). \tag{4.7}$$

From the point of view of validating the theory, the important point to note is that the change in external electronic energies is only equivalent to (4.7) if it is valid to ignore such energy changes in impurity excitation lines such as (2.12*b*) and (2.12*c*).

Diagrams evaluated with the modified propagators are equivalent to the sum of the vertex functions that results from writing

$$\frac{\mathrm{i}}{(\omega^{\pm} - \mu - k)} = \frac{\mathrm{i}}{(\omega^{\pm} - k)} - \int_0^{\mu} \mathrm{d}\omega' \frac{\mathrm{i}}{(\omega^{\pm} - \omega' - k)^2} \tag{4.8}$$

and then expanding in powers of the integration operation. Taking the momentum integral gives

$$\int_0^{\Lambda} \mathrm{d}k \qquad \text{or} \qquad \int_{-\Lambda}^{0} \mathrm{d}k \frac{(-\mathrm{i})}{(\omega^{\pm} - \omega' - k)^2} = \frac{\pm \mathrm{i}}{(\omega^{\pm} - \omega')} \mp \frac{\mathrm{i}}{(\omega^{\pm} - \omega' \mp \Lambda)} \tag{4.9}$$

where the upper sign applies in the case of a particle line and the lower sign for a hole line. On taking the integral over the Feynman energy loop variable, the first term in (4.9) causes the associated external electron lines to acquire the external energy ω'. The second term in (4.9) makes this external energy to be of the order $\pm\Lambda$, and this alters the asymptotic part which is yet to be taken. In diagrams with $D < 0$ an external energy of the order of Λ implies a zero asymptotic contribution, and for self-energy diagrams with $D = 1$ any finite contribution can be absorbed into the renormalised mass of equation

(3.6). The net result is that to each integration operation there is a pair of contracted external electron legs with external energy ω', which the integration operation integrates from 0 to μ.

The final series for the vertex function with external energies $\omega_e - \mu$ is identical to what one would get by calculating the scattering of the original electrons with energy ω_e in the presence of a whole set of additional electrons that just raise the fermi level from 0 to μ. As Nozieres has stressed, the Kondo properties are tied to the fermi level, and so this is the point from which the electronic energies should be measured.

It is hard to see how these Ward identities could remain valid if the asymptotic part of the impurity excited states, such as (2.12*b*) and (2.12*c*), was taken in some other way.

5. Alternative Hamiltonians belonging to the same field theory

In this section we show that the original Hamiltonian (1.1) with J anti-ferromagnetic, impurity spin $S > \frac{1}{2}$, and the interaction term

$$-J\boldsymbol{S}_e \cdot \boldsymbol{S} = -J \int \mathrm{d}k \int \mathrm{d}k' c_k^\dagger \boldsymbol{S}_e c_{k'} \cdot \boldsymbol{S}, \tag{5.1a}$$

can give rise to a field theory that is identical to the field theory produced by a Hamiltonian with K ferromagnetic, impurity spin $S' = S - \frac{1}{2}$, and the interaction term

$$-K\boldsymbol{S}_e \cdot \boldsymbol{S}' = -K \int \mathrm{d}k \int \mathrm{d}k' \, q_k^\dagger \boldsymbol{S}_e q_{k'} \cdot \boldsymbol{S}'. \tag{5.1b}$$

The Ward integral equations for the alternative expansion of (5.1*a*) have identically the same structure as the Ward integral equations for the standard expansion of (5.1*b*), and vice versa. This immediately implies that the two field theories must be identical if the two renormalised exchange constants involved have the same numerical value at the same renormalisation point.

The Hamiltonian terms (5.1) are true energy-independent Hamiltonian terms, and so the relationship between them must be independent of the renormalisation point energy ω_R. Identical Ward equations imply identical renormalisation-group equations, and this in turn implies that if the renormalised exchange constants are equal at one renormalisation point, then they must be equal at any other renormalisation point. If the asymptotic expressions are equated at $\omega_R = -\Lambda$ then the logarithmic terms, such as in (3.13), disappear.

The alternative expansion applied to Hamiltonian (5.1*a*) gave equation (3.13), whereas the standard expansion applied to Hamiltonian (5.1*b*) gives

$$K_R(\omega_R) = K + K^2 \ln(-\omega_R/\Lambda) + \ldots. \tag{5.2}$$

Hence an identical field theory will result from both this Hamiltonian and from (5.1*a*) if this renormalised exchange constant has the same value as that given by (3.13), i.e. the two Hamiltonians are equivalent if

$$K = \left(\frac{-8}{\pi^2(2S+1)} \frac{1}{J(S+1)}\right) + C_2\left(\frac{-8}{\pi^2(2S+1)} \frac{1}{J(S+1)}\right)^2 + \mathrm{O}\left(\frac{1}{J^3}\right). \tag{5.3}$$

The large-K expansion of this equivalence relation may be found by making the

alternative expansion on (5.1*b*) instead of on (5.1*a*). This gives

$$J=\left(\frac{-8}{\pi^2(2S'+1)}\frac{1}{KS'}\right)+C_2\left(\frac{-8}{\pi^2(2S'+1)}\frac{1}{KS'}\right)^2+\mathrm{O}\left(\frac{1}{K^3}\right). \tag{5.4}$$

The alternative Hamiltonian is not unique. If (5.1*a*) had been mapped onto a Hamiltonian with the interaction term

$$-\bar{K}\int \mathrm{d}k\int \mathrm{d}k'\,\Gamma(k)q_k^{\dagger}\boldsymbol{S}_{\mathrm{e}}q_{k'}\Gamma^*(k')\cdot\boldsymbol{S}' \tag{5.5}$$

instead of the interaction term (5.1*b*), then an equivalent field theory is again obtained if the Hamiltonian coefficients are now related by

$$\bar{K}=\left(\frac{-8}{\pi^2(2S+1)}\frac{1}{J(S+1)}\right)+\mathrm{O}\left(\frac{1}{J^3}\right). \tag{5.6}$$

In this case the second-order term is identically zero. The second-order term is also usually zero in the numerical calculations reported below, for the same reason that it is zero here.

All of the theory of this paper can also be applied to Wilson's (1974) Hamiltonian

$$H=-J\chi^{N-1}f_0^{\dagger}\boldsymbol{S}_{\mathrm{e}}f_0\cdot\boldsymbol{S}+\sum_{j=1}^{N}\chi^{N-j}(f_j^{\dagger}f_{j-1}+f_{j-1}^{\dagger}f_j). \tag{5.7}$$

Although this is a discrete eigenvalue problem, equivalent to a $(2S+1)4^{N+1}\times(2S+1)4^{N+1}$ matrix diagonalisation problem, it also possesses a 'field theory' that satisfies renormalisation equations just as with the previous continuum Hamiltonians. These equations now show that the many-particle eigenvalues are not functions of the iteration number N and the exchange constant J separately, but are actually functions of the combination

$$N-N_{\mathrm{K}}(J), \tag{5.8}$$

with all the J dependence of the theory entering through the 'Kondo number' $N_{\mathrm{K}}(J)$. The asymptotic part of the Hamiltonian theory is here obtained by dropping all terms of order χ^{-N} that are not of the form (5.8). The many-particle eigenvalues of this Hamiltonian can be found by an iterative numerical technique, as has been used by Wilson (1974, 1975), Krishna-murthy *et al* (1975, 1977, 1980), Cragg and Lloyd (1978, 1979a, b) and Cragg *et al* (1980). These calculated eigenvalues attain their 'field-theory values' once the iteration number N is sufficiently large so that the initial transients, corresponding to the terms of order χ^{-N}, have died out.

The theory of this section predicts that the many-particle eigenvalues of (5.7) will be, after the initial transients have died out, identical to those of the Hamiltonian

$$H=-K\chi^{N-2}g_0^{\dagger}\boldsymbol{S}_{\mathrm{e}}g_0\cdot\boldsymbol{S}'+\sum_{j=1}^{N-1}\chi^{N-1-j}(g_j^{\dagger}g_{j-1}+g_{j-1}^{\dagger}g_j), \tag{5.9}$$

which has one less iteration than (5.7), providing that $S'=S-\frac{1}{2}$ and that the ferromagnetic K-value is suitably related to the anti-ferromagnetic J-value. Alternatively, the many-particle eigenvalues of the ferromagnetic Hamiltonian

$$H=-K\chi^{N-1}f_0^{\dagger}\boldsymbol{S}_{\mathrm{e}}f_0\cdot\boldsymbol{S}'+\sum_{j=1}^{N}\chi^{N-j}(f_j^{\dagger}f_{j-1}+f_{j-1}^{\dagger}f_j) \tag{5.10}$$

can be made the same as those of the anti-ferromagnetic Hamiltonian

$$H = -J\chi^{N-2} g_0^\dagger \boldsymbol{S}_e g_0 \cdot \boldsymbol{S} + \sum_{j=1}^{N-1} \chi^{N-1-j} (g_j^\dagger g_{j-1} + g_{j-1}^\dagger g_j), \tag{5.11}$$

again with one less iteration. That any of these Hamiltonians maps onto a similar one, but with two less iterations, is a consequence of (5.8). In perturbation theory, the transients are proportional to the smaller exchange constant squared, and so for numerical investigations it is better to map (5.7) onto (5.9) when $(-J) > K$, and to map (5.10) onto (5.11) when $K > (-J)$.

These equations have been explored numerically with $S = 1$, $S' = \frac{1}{2}$, $\chi^3 = 3$. By making several calculations with different values of J and K, it has always been possible to find related pairs of J- and K-values such that both sets of many-particle eigenvalues agree once the initial transients have died out. With a large ferromagnetic K, the calculated eigenvalue curves are the same as those displayed in Cragg and Lloyd (1979b) as an example of a small anti-ferromagnetic exchange constant calculation. In this case both sets of calculated eigenvalues become identical (to within numerical error) well before the cross-over, and remain identical right through the cross-over and on up to the fixed point. For the reasons discussed in the last paragraph, the initial transients decay slowest when $(-J) \sim K$, and some calculated values for this case are given in table 1. These values start from about half way through the cross-over of the figure in Cragg and Lloyd (1979b). This is a 'worst case' example. When $J \sim -0{\cdot}2$ the differences at the same iteration number are smaller by a factor of about 50, and when $J \sim -0{\cdot}02$ they are smaller by a factor of about 5000.

Table 1. Some many-particle excitation energies as measured from the lowest $S = \frac{1}{2}$ state, labelled by their total spin S, as a function of the iteration number N. The even-N values have been calculated from Hamiltonian (5.11) with $J = -2{\cdot}246\,15$, and the odd-N values have been calculated from Hamiltonian (5.10) with $K = +2{\cdot}37$. As discussed in the text, this is a 'worst case' example. The differences between the two calculations decay as χ^{-N}, and by $N = 20$ both sets agree to five figures.

N \ S	1	0	$\frac{3}{2}$	$\frac{1}{2}$
2	0·797 49	1·299 18	1·499 50	1·939 06
3	0·733 92	1·192 46	1·415 36	1·746 50
6	0·737 15	1·014 97	1·449 56	1·632 44
7	0·731 23	1·006 79	1·440 96	1·616 19
10	0·748 84	0·949 92	1·487 58	1·604 29
11	0·748 17	0·949 08	1·486 59	1·602 54

The above numerical results appear to confirm that for each J there is a definite K that produces the same many-particle eigenvalues. Calculations have also been made to try to check the specific analytic relationship. The theory shows that for large J (5.7) maps onto (5.9) if

$$K = -\chi\left[\frac{8}{(2S+1)}\frac{1}{J(S+1)} + \frac{128(2S+1)+32}{(2S+1)^3}\left(\frac{1}{J(S+1)}\right)^3 + \mathrm{O}\left(\frac{1}{J^4}\right)\right] \tag{5.12}$$

and that for large K (5.10) maps onto (5.11) if

$$J = -\chi\left[\frac{8}{(2S'+1)}\frac{1}{KS'} + \frac{-128(2S'+1)+32}{(2S'+1)}\left(\frac{1}{KS'}\right)^3 + O\left(\frac{1}{K^4}\right)\right]. \tag{5.13}$$

With $S = 1$, $S' = \frac{1}{2}$, $\chi^2 = 3$ this latter equation is

$$J = -\sqrt{3}[8/K - 224/K^3 + O(1/K^4)]. \tag{5.14}$$

To test this a series of calculations have been made, with typical results being: a $K = 100$ calculation gave the same eigenvalues as $J/\chi = 0{\cdot}079\,768$ while (5.14) gives $J/\chi = -0{\cdot}079\,776$; a $K = 400$ calculation is equivalent to a $J/\chi = -0{\cdot}019\,9965$ one, which is also the value given by (5.14). Numerically it appears that equivalent J-values can be determined with extraordinary accuracy. Over many iterations all the lower eigenvalues could be brought into coincidence up to the eighth decimal place. This is much more accurate than the eigenvalues themselves. Halving the number of states retained at each iteration alters the eigenvalues in the fourth decimal place, but the J and K calculations altered similarly, maintaining the agreement between the two at the eighth decimal place. Taking such calculated J-values at their face value, they could be fitted to

$$J/\chi + 8/K - 224/K^3 = (700 \pm 100)/K^4 + a\ e^{bK}, \tag{5.15}$$

with $a = 3\times10^{-9}$ and $b = 4\times10^{-3}$ accurate to about a factor of two. The first term on the right of (5.15) has the expected form, but the second does not. This latter term only contributes at extremely large K-values, and we believe that it is spurious and due to some non-understood feature of the numerical approximations.

The third order in the $1/K$ contribution being tested comes from: the modification of the first-order diagrams (2.16) due to the change in energy (2.3) by the self-energy diagrams

 (5.16)

the differentials of these diagrams that give a contribution through the Z factor that multiplies the first-order diagrams; diagrams like (2.20) but with an excited intermediate state; and from the energy dependence of the diagrams (2.20) themselves, as discussed in the first paragraph of § 3. Inasmuch as the calculations validate the third-order term, it is only validating these contributions.

6. The ferromagnetic spin-zero impurity

In this section it is shown that the alternative Hamiltonian theory can also be applied to the symmetric Anderson (1961) Hamiltonian, and that it maps it onto the antiferromagnetic spin-$\frac{1}{2}$ Kondo Hamiltonian.

The previous discussion maps a ferromagnetic spin-S' Hamiltonian onto an antiferromagnetic spin-$S = S' + \frac{1}{2}$ Hamiltonian. An anti-ferromagnetic spin-$\frac{1}{2}$ Hamiltonian should therefore follow from the ferromagnetic Hamiltonian

$$H = -2\Lambda K f^\dagger \boldsymbol{S}_e f \cdot \boldsymbol{S}' + \sqrt{\Lambda}\Gamma \int (q_k^\dagger f + f^\dagger q_k)\,\mathrm{d}k + \int k q_k^\dagger q_k\,\mathrm{d}k \tag{6.1}$$

in the limit $S' \to 0$. In fact, mapping this Hamiltonian onto

$$H = -J \int \mathrm{d}k \int \mathrm{d}k'\, q_k^\dagger \boldsymbol{S}_e q_{k'} \cdot \boldsymbol{S} + \int k q_k^\dagger q_k \,\mathrm{d}k, \tag{6.2}$$

with $S = S' + \frac{1}{2}$, gives the equivalence relation

$$J = -\frac{4}{(2S'+1)}\frac{\Gamma^2}{KS'} + \frac{32(2S'+1)-8}{(2S'+1)^3}\frac{\Gamma^4}{(KS')^3} + \ldots, \tag{6.3}$$

and so such a limit only exists if the ferromagnetic exchange constant is itself a function of S' of the form

$$K = U/S'. \tag{6.4}$$

In forming the alternative expansion for (6.1), the energy E_- of equation (2.3),

$$E_- = \Lambda(S'+1)U/S', \tag{6.5}$$

becomes infinite in this limit. Consequently this state is effectively suppressed from the Hilbert space. On the other hand

$$E_+ = -\Lambda U \tag{6.6}$$

is finite in the limit $S' \to 0$. The relevant zero-particle, two-particle and E_+ spin-$\frac{1}{2}$ states of the impurity centre are then identical to the eigenstates of

$$H_A = 2\Lambda U[(n_\uparrow - \tfrac{1}{2})(n_\downarrow - \tfrac{1}{2}) - \tfrac{1}{4}] \qquad \text{with } n_\sigma = f_\sigma^\dagger f_\sigma. \tag{6.7}$$

Equation (6.7) is the interaction term in the symmetric Anderson model, where it describes the repulsive electron–electron interaction on the local impurity site.

The symmetric Anderson Hamiltonian is

$$H = H_A + \sqrt{\Lambda}\Gamma \int (q_k^\dagger f + f^\dagger q_k)\,\mathrm{d}k + \int k q_k^\dagger q_k \,\mathrm{d}k. \tag{6.8}$$

This is already in the transformed form of equation (2.8) from which the alternative expansion was developed. The analogue of the original Hamiltonian (1.1) is the Wolff (1961) Hamiltonian, and the transformation between the two as given in § 2 is the same as was used by Lloyd and Osborne (1971) to relate these models.

The diagrammatic rules for the alternative expansion of the Anderson Hamiltonian can be cast into an almost identical form to the rules given in § 2. With the − state no longer existing, the + state of (2.12*a*) is now the only one-electron impurity state, and its energy is given by (6.6). If a suitable phase convention is chosen, the rest of the rules are then identical to those of § 2, with the exception that the vertex factor of (iii) is now $\sqrt{\Lambda}\Gamma$ and that the Clebsch–Gordan coefficients must be interpreted as being

$$C_\sigma^+(M) = \mathrm{sgn}(\sigma), \qquad C_\sigma^-(M) = 0. \tag{6.9}$$

Conservation of the z component of spin implies that the only Clebsch–Gordan coefficients that actually occur in the diagrams are $C_\sigma^\pm(-\sigma)$. For these, the formulae (2.5) for the Clebsch–Gordan coefficients do actually give the values of equation (6.9) when evaluated with the spin being zero. Moreover, the analogue of (2.17) for ferromagnetic spin $S' = S - \frac{1}{2}$ is

$$C_{\sigma'}^+(M')C_\sigma^+(M) = \tfrac{1}{2}\delta_{M'M}\delta_{\sigma'\sigma} - \frac{2}{2S'+1}[\boldsymbol{S}_e]_{\sigma'\sigma} \cdot [\boldsymbol{S}]_{M'M} \tag{6.10a}$$

$$\operatorname{sgn}(\sigma)C^{+}_{-\sigma}(M')\operatorname{sgn}(\sigma')C^{+}_{-\sigma'}(M) = \tfrac{1}{2}\delta_{M'M}\delta_{\sigma'\sigma} + \frac{2}{2S'+1}[\boldsymbol{S}_e]_{\sigma'\sigma}\cdot[\boldsymbol{S}]_{M'M} \qquad (6.10b)$$

and these equations are still valid when evaluated with (6.9) if one also substitutes $S' = 0$, and takes $\boldsymbol{S}$ to be a spin-$\frac{1}{2}$ operator. The example at the end of § 2 now translates into an example to show how the Anderson model produces an effective anti-ferromagnetic spin-$\frac{1}{2}$ scattering centre.

The alternative expansion for the Anderson model can be renormalised as in § 3, and by following § 5 the Anderson model can be mapped onto the anti-ferromagnetic spin-$\frac{1}{2}$ Hamiltonian of equation (6.2). The two Hamiltonians give rise to identical field theories if

$$J = -4\Gamma^2/U + 24\Gamma^4/U^3 + \ldots. \qquad (6.11)$$

As can be seen, this is the $S' \to 0$ limit of (6.3) after the exchange constant has been put into the form (6.4).

We have not investigated this relation numerically. But Krishna-murthy *et al* (1980) have investigated the Anderson Hamiltonian by means of Wilson-style calculations in great detail, and we refer the reader to their paper. These authors comment on the wide range of applicability of the Schrieffer–Wolff (1966) transformation, i.e. the first term in (6.11). Presumably, this is because there is no second-order term in the expansion (6.11).

7. Discussion

In a particle physics problem, relativistic invariance demands that the cut-off be a true infinite quantity. This contrasts with a solid-state physics problem where the cut-off always has some real physical interpretation and is finite. Indeed, in real Kondo materials this 'infinite cut-off' only has a magnitude of about one electron volt! For this reason it is almost essential to think of the field theory of such a problem as being the asymptotic part to the given Hamiltonian theory. In a Kondo system the thermal energies of interest are of the order of $10^{-4}\Lambda$ and so any corrections to the field theory solution are of the order of about 0·01%.

Both strong and weak asymptotic forms may exist. In terms of the Kondo problem, the strong asymptotic assumption corresponds to the particle physics limit $\Lambda \to \infty$ $J \to 0$ with E_K fixed. If Λ is finite this corresponds to the assumption that J, which is of the order of $1/\ln(\Lambda)$, is also negligible. However, the direct application of the renormalisation program, say by means of the Ward integral equations, can be equivalent to a weaker asymptotic assumption than this. An example of this occurs in Cragg and Lloyd (1978, 1979a), who considered the effect of a scattering potential term on the Kondo problem. Under the strong asymptotic assumption, the resultant total phase shift is then just the sum of the individual phase shifts due to the potential and spin terms separately, but a weaker asymptotic limit can also be derived from the renormalisation equations in which there are small corrections to this peculiar result.

The renormalised field theory is fully parametrised by the inhomogeneous terms in the Ward integral equations. In particle physics these are usually taken as being arbitrary, even when there is no corresponding bare term in the original Lagrangian. However, in a solid-state physics problem these renormalised parameters are the repositories of the original Hamiltonian parameters and are fully determined by the Hamiltonian.

These renormalised parameters may turn out to be 'infinite' as far as the asymptotic part to the Hamiltonian theory is concerned (say of order Λ). The renormalisation procedure is not always unique, and in the present problem each vertex (2.14) and each excited state of the impurity could be separately renormalised, as would be done if each of these were separate new particles. This, though, produces a large number of such parameters with no obvious relationships between them, and it is known that the true asymptotic form depends only on the single Kondo energy parameter. It is possible that each of these are actually functions of the Kondo energy only, but the authors believe that they are 'infinite' quantities and that ratios of the mass and vertex terms are needed in order to produce 'finite' quantities, and that the renormalisation used in the text is correct.

The Hamiltonian only determines a unique field theory if an order of magnitude for the various Hamiltonian terms has been specified. As the parameters in the Anderson Hamiltonian (6.8) have been defined in terms of the magnitude of the cut-off, this Hamiltonian already incorporates such a specification. A different set of orders of magnitude for the terms could have been considered, and perhaps the specification given in (6.8) is more in the spirit of the Wolff model than of the Anderson model. The recent important studies of the Anderson Hamiltonian by Yosida and Yamada (1970, 1975), Yamada (1975a, b), Yoshimori (1976) and Haldane (1978) feature a limit in which the electron–electron repulsive energy remains finite as the conduction band width tends to infinity. This is a quite different assumption from that which is implicit in writing the repulsive energy as $U\Lambda$, and it gives rise to quite a different asymptotic theory. In this theory the relevant electronic energies can exceed the repulsive energy, and so it is not always equivalent to a spin-$\frac{1}{2}$ Kondo Hamiltonian but also includes a free orbital regime. Even where it is equivalent to a spin-$\frac{1}{2}$ impurity, dimensional arguments show that the third-order term in (6.11) is no longer correct.

On the other hand, the numerical Hamiltonian studied by Krishna-murthy *et al* (1975, 1977, 1980) is the analogue of the Anderson Hamiltonian (6.8), with $\Lambda = \chi^{N-1}$ and the conduction band made discrete. But, here also it is possible to select the Hamiltonian parameters and the iteration number such that the initial transients have already died out even though the energies of interest are still greater than $U\Lambda$. The analogue of the relation (6.11) between the Anderson Hamiltonian and the exchange constant (but as calculated for the discrete Hamiltonian) will not then apply until the iteration number is such that $U\chi^{N-1}$ is also much larger than the calculated eigenvalues. In the application of any asymptotic theory, one must always be sure that the appropriate asymptotic limit is being applied.

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