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1970 J. Phys. C: Solid State Phys. 3 2436

(http://iopscience.iop.org/0022-3719/3/12/008)

J. Phys. C: Solid St. Phys., 1970, Vol. 3. Printed in Great Britain

A poor man's derivation of scaling laws for the Kondo problem

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MS. received 28th April 1970

Abstract. The scaling laws derived by a complicated space-time approach for the Kondo problem in previous work are rederived by a 'cutoff renormalization' technique used previously in the theory of superconductivity.

In a series of recent papers (Anderson and Yuval 1969, 1970, Anderson *et al.* 1970a, b) we showed the equivalence of an anisotropic Kondo problem to a certain kind of one dimensional statistical problem, and solved that problem by deriving scaling laws connecting solutions for different sets of parameters with each other, and specifically with one or another soluble case.

Here we show that these scaling laws are derivable directly and easily in the Kondo problem itself. As in the previous work, the solution of the ferromagnetic case becomes trivial, but the antiferromagnetic one may require, for some purposes, solution of an auxiliary problem. As in previous methods, the parameters of the auxiliary problem are not perfectly defined, but it is clear that that solution behaves like a simple bound state with no singular properties.

The method is based on a technique used in the theory of the 'Coulomb pseudopotential' in superconductivity (Morel and Anderson 1962, Schrieffer 1964). In that problem it was convenient to confine one's interest to the region within a Debye energy of the Fermi surface so what was done was to calculate an effective interaction or 'pseudopotential' which was equivalent, acting in this limited region of momentum space, to the real potential in the full region. Here our technique will be the same: to eliminate successively the higher energy regions in favour of an effective interaction.

Consider the Dyson equation for the scattering matrix T

$$T(\omega) = V_{\rm int} + V_{\rm int}\, G_0(\omega)\, T(\omega) \tag{1}$$

where

$$V_{\rm int} = \frac{J_\pm}{2}(S_+ s_- + S_- s_+) + J_z S_z s_z \tag{2}$$

is the anisotropic Kondo interaction. ($S_\pm = S_x \pm iS_y$). G_0 is the unperturbed Green function for propagation of free electrons in the band

$$G_0 = (\omega - \mathscr{H}_0)^{-1} \tag{3}$$

$$\mathscr{H}_0 = \sum_{\epsilon_k = E_F - E_c}^{E_F + E_c} \epsilon_k n_{k\sigma} \tag{4}$$

† Work at the Cavendish Laboratory supported in part by the Air Force Office of Scientific Research Office of Aerospace Research, US Air Force, under Grant Number 1052-69.

and for simplicity this band is assumed symmetric about the Fermi surface with a sharp cutoff at E_c.

(1) is the exact definition of the matrix T, which is not assumed to have single particle scattering character or any other limitation. We are interested in ω near the ground state in energy, so not a great many excited particles will in fact be present. It is an exact identity that

$$G = G_0 + G_0 T G_0 \tag{5}$$

and the lowest pole of G, and thus of T, determines the ground state. G is here *not* a many body Green function in the usual Matsubara sense but the actual resolvent operator $(\omega - \mathscr{H})^{-1}$.

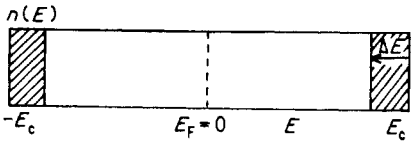

Figure 1.

We now attempt to reduce the cutoff energy E_c to $E_c - \Delta E$, $\Delta E \ll E_c$. (see figure 1). States near E_c are not highly occupied in the ground state and ΔE is arbitrarily small, so it is certainly rigorous to study only states with few or no excited electrons k'' with $E_c > |\epsilon_{k''}| > E_c - \Delta E$ (we shift energy zero to $E_F = 0$). We now try to take into account explicitly all scatterings from our low energy state of interest into $E_c > \epsilon_{k''} > E_c - \Delta E$ by introducing a projection operator $P_{\Delta E}$ which projects *on to states containing one or more such particles.* We then simply resolve (1)

$$T = V + V P_{\Delta E} G_0 T + V(1 - P_{\Delta E}) G_0 T$$

and resubstituting (1) in the second term we get

$$\begin{aligned} T &= V + V P_{\Delta E} G_0 V + (V + V P_{\Delta E} G_0 V)(1 - P_{\Delta E}) G_0 T + V P_{\Delta E} G_0 V P_{\Delta E} G_0 T \\ &= V' + V'(1 - P_{\Delta E}) G_0 T \end{aligned} \tag{6}$$

where

$$V' = V + V P_{\Delta E} G_0 V. \tag{7}$$

In getting (6) we have neglected (relative to 1)

$$V P_{\Delta E} G_0 V P_{\Delta E} G_0 \simeq (\Delta E)^2 \rho^2(E) V^2 / E_c^2 \tag{8}$$

which is proportional to $(\Delta E)^2$ and may thus be made small.

Equations (5), (6) and (7) are equivalent to the statement that the original problem with cutoff at E_c is exactly (to order $(\Delta E)^2$) equivalent to a new problem in which, according to (6), we may cut out all matrix elements of T (and therefore of V) leading into the ΔE subspace. By multiplying (6) by $(1 - P)$ on the left and right, we eliminate all matrix elements outside the new cutoff, and have a complete new physical problem as far as matrix elements of G within the remaining subspace are concerned. The new potential V', according to (7), is changed from V by an amount

$$\mathrm{d}V = V P_{\Delta E} G_0 V \tag{9}$$

proportional to ΔE (The projection operators $(1 - P)$ on the left and right may be understood of course.).

Clearly if we can evaluate (9) we are left with a new problem to which the same trick may be applied and in the end we get a differential equation relating sets of equivalent problems. Let us then insert (2) in (9). Formally,

$$dV = \sum_{k_1,\sigma_1}^{|\epsilon_{k_1}|<E_c-\Delta E} \sum_{k_2,\sigma_2}^{|\epsilon_{k_2}|<E_c-\Delta E} \sum_{k,\sigma}^{E_c>|\epsilon_k|>E_c-\Delta E} \frac{1}{\omega - E_c - |\epsilon_{k_1}|}$$

$$\times \left[(C^+_{k_2\sigma_2} C_{k\sigma})(C^+_{k\sigma} C_{k_1\sigma_1}) \left\{ \frac{J_\pm}{2}(S_+(s_-)_{\sigma_2\sigma} + S_-(s_+)_{\sigma_2\sigma}) + J_z S_z (s_z)_{\sigma_2\sigma} \right\} \right.$$

$$\times \left\{ \frac{J_\pm}{2}(S_+(s_-)_{\sigma\sigma_1} + S_-(s_+)_{\sigma\sigma_1}) + J_z S_z (s_z)_{\sigma\sigma_1} \right\} + C^+_{k\sigma} C_{k_2\sigma_2} C^+_{k_1\sigma_1} C_{k\sigma} \left\{ \frac{J_\pm}{2}(S_+(s_-)_{\sigma\sigma_2} \right.$$

$$\left. \left. + S_-(s_+)_{\sigma\sigma_2}) + J_z S_z (s_z)_{\sigma\sigma_2} \right\} \left\{ \frac{J_\pm}{2}(S_+(s_-)_{\sigma_1\sigma} + S_-(s_+)_{\sigma_1\sigma}) + J_z S_z (s_z)_{\sigma_1\sigma} \right\} \right].$$

This formidable expression has already had some simplifications carried out. It is assumed that k_1 is not excited in the initial state in order to insert $|\epsilon_{k_1}|$; ΔE is small so $|\epsilon_k| \simeq E_c$, and we know k is unexcited. Actually the number of excited particles is relatively $\simeq 1/\text{total volume} \ll 1$.

To further simplify we set $C^+_{k\sigma} C_{k\sigma} = 1$ or 0 for k below or above the Fermi sea, and sort out the algebra of the s by summing over σ and using

$$s_+ s_- = \tfrac{1}{2} + s_z \qquad s_- s_+ = \tfrac{1}{2} - s_z$$

$$s_- s_z = -s_z s_- = \tfrac{1}{2} s_- \qquad s_+ s_z = -\tfrac{1}{2} s_+ = -s_z s_+$$

$$s_z s_z = \tfrac{1}{4}$$

(specializing also to $|S| = \frac{1}{2}$). This gives us

$$dV = \sum_{k_1,\sigma_1} \sum_{k_2,\sigma_2} \frac{\rho \Delta E}{\omega - E_c - |\epsilon_{k_1}|} \left[C^+_{k_2\sigma_2} C_{k_1\sigma_1} \left\{ \delta_{\sigma_1\sigma_2} \left(\frac{J^2_\pm}{8} + \frac{J^2_z}{16} \right) - \frac{J^2_\pm S_z (s_z)_{\sigma_2\sigma_1}}{2} \right. \right.$$

$$\left. - \frac{J_\pm J_z}{4}(S_+(s_-)_{\sigma_2\sigma_1} + S_-(s_+)_{\sigma_2\sigma_1}) \right\} + C_{k_2\sigma_2} C^+_{k_1\sigma_1} \left\{ \delta_{\sigma_1\sigma_2} \left(\frac{J^2_\pm}{8} + \frac{J^2_z}{16} \right) + \frac{J^2_\pm S_z (s_z)_{\sigma_1\sigma_2}}{2} \right.$$

$$\left. \left. + \frac{J_\pm J_z}{4}(S_+(s_-)_{\sigma_1\sigma_2}) \right\} \right]. \tag{10}$$

The reason for the solubility of the Kondo problem is that (10) has virtually the same form as (2). To reduce it to exactly the same form we have to make some approximations. First a very good one: the $\delta_{\sigma_1\sigma_2}$ terms for $k_1 \neq k_2$ are simply

$$\frac{1}{16}(J_z^2 + 2J_\pm^2) C^+_{k_1\sigma_1} C_{k_2\sigma_1} \rho \Delta E \left\{ \frac{|\epsilon_{k_1}| - |\epsilon_{k_2}|}{(\omega - E_c - |\epsilon_{k_1}|)(\omega - E_c - |\epsilon_{k_2}|)} \right\} \tag{11}$$

which is an ordinary scattering potential which is small, and actually zero at the Fermi surface and on the average. Clearly (11) will not contribute significantly to the infrared divergences which are the heart of the Kondo problem, so hereafter we neglect it. The $k_1 = k_2$ terms, however, lead to a significant result

$$dV_0 = \frac{\rho \Delta E}{8}(J_z^2 + 2J_\pm^2) \sum_{\epsilon_k = 0}^{E_c} (\omega - E_c - |\epsilon_k|)^{-1}. \tag{12}$$

This term is not of a form similar to the unperturbed Hamiltonian; it is simply a constant number, a shift of the zero of the energy scale. It represents the net shift of total ground state energy due to scatterings into the ΔE subspace. It would be perfectly consistent to retain it by adding a constant to the interaction V but it is more convenient to incorporate it in $\mathcal{H}_0$ and thus in G_0 at each stage

$$\mathcal{H}'_0 = \mathcal{H}_0 + dV_0$$

$$G'_0 = (\omega - \mathcal{H}_0 - dV_0)^{-1}.$$

Since dV_0 is simply a numerical constant (not a particle selfenergy!) it has no effect to include this ground state energy change except to redefine ω. Thus we may sum up the total ground state energy shift at any stage as

$$\Delta(E_g) = \int_{E_c}^{E_c^0} dE \left(\frac{(J_z\rho)^2}{8} + \frac{(J_\pm\rho)^2}{4}\right) \ln\left(\frac{2E - \omega - \Delta}{E - \omega - \Delta}\right) \simeq \ln 2 \int_{E_c}^{E_c^0} \left(\frac{(J_z\rho)^2}{8} + \frac{(J_\pm\rho)^2}{4}\right) dE. \tag{13}$$

This is the first of the scaling laws and corresponds to (15) of our previous paper (Anderson *et al.* 1970).

We are left with the spin dependent terms. The simplest and most important case occurs when $J\rho \ll 1$. If we look back at (8) we will see that the limit on $\Delta E/E_c$ is set by $1/J\rho$. If ΔE may be set fairly large (we call this 'renormalization by leaps and bounds') the relevant values of $|\epsilon_{k_1}|$ are small compared with E_c, and it may be very accurately stated that

$$\frac{dV}{\Delta E} = \frac{\rho}{\omega - E_c + \Delta(E_c)} \sum_{k_1\sigma_1 k_2\sigma_2} C^+_{k_2\sigma_2} C_{k_1\sigma_1} \Big\{ -J_\pm^2 S_z (s_z)_{\sigma_2\sigma_1} - \frac{J_\pm J_z}{2} (S_+(s_-)_{\sigma_2\sigma_1} + S_-(s_+)_{\sigma_2\sigma_1}) \Big\}.$$

This equation shows that the change in the effective perturbation V which is caused by changing the cutoff energy E_c by a small amount is formally equivalent to an anisotropic exchange interaction, and so the effect is merely to change the parameters of the original interaction. This is why we call the procedure 'scaling laws', because what we have done is to show that a problem with one set of parameters is entirely equivalent to that with another set. This leaves us with the hope, usually fulfilled, that by following the scaling procedure out repeatedly we can eventually reach a region where a solution by some other method may be found. The differential equations connecting the three parameters E_c, J_z and $J_\pm$ are, then,

$$\frac{dJ_z}{dE_c} = -\frac{\rho}{\omega - E_c + \Delta} J_\pm^2 \tag{14}$$

$$\frac{dJ_\pm}{dE_c} = -\frac{\rho}{\omega - E_c + \Delta} J_z J_\pm. \tag{15}$$

These are the two primary scaling laws corresponding to (18) and (21) of the previous paper (Anderson *et al.* 1970). The most important conclusion is obtained by dividing (14) by (15) and integrating the resulting equation to obtain

$$J_z^2 - J_\pm^2 = \text{const} \tag{16}$$

the set of hyperbolic curves connecting different cases in the neighbourhood of the origin (see figure 2). Equation (16) shows that ferromagnetic cases on or to the right of the isotropic line are solved trivially by scaling to $J_\pm = 0$, as discussed previously and in agreement with Mattis' general theorem (Mattis 1967)† and with the results of Shiba (preprint). All antiferromagnetic cases with $J\rho \ll 1$, and ferromagnetic cases on the antiferromagnetic side of the isotropic line, scale *away* from small J in the end, and, no matter how weak the original coupling, eventually become equivalent to large $J\rho$. (Note that the sign of (14) shows that J_z always increases; ferromagnetic is J_z negative; while (15) changes sign at $J_z = 0$.) Fuller implications of the scaling laws for small J, especially in regard to the Ising model, are being presented elsewhere.

† Dr Mattis has kindly shown us a generalization to anisotropic exchange which shows that the ferromagnetic isotropic case is indeed the boundary.

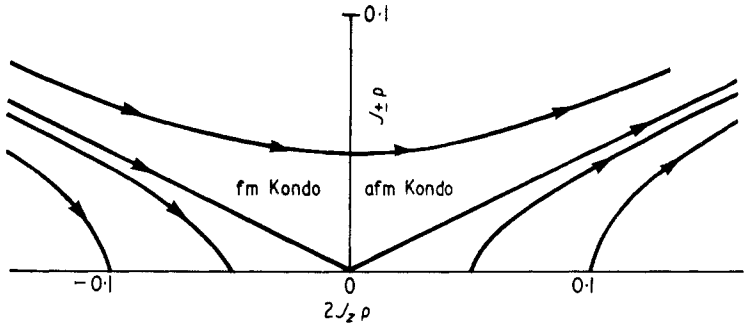

Figure 2.

The interesting antiferromagnetic case, as shown by our previous work, is unfortunately the case in which, as E_c decreases, (14) and (15) become less accurate. In this case the ω and k dependence in (10) becomes increasingly less negligible. Leaving that dependence in, we obtain

$$dV = -\rho\Delta E \sum_{k_1\sigma_1 k_2\sigma_2} \left\{ \frac{J_\pm^2}{2} S_z (s_z)_{\sigma_2\sigma_1} - \frac{J_\pm J_z}{4} (S_+ (s_-)_{\sigma_2\sigma_1} + S_- (s_+)_{\sigma_2\sigma_1}) \right\} \times \left\{ \frac{1}{\omega - E_c + \Delta - |\epsilon_{k_1}|} + \frac{1}{\omega - E_c + \Delta - |\epsilon_{k_2}|} \right\} C^+_{k_2\sigma_2} C_{k_1\sigma_1}. \tag{16}$$

Since in general the denominators are negative, this means that the increase in J is slightly greater at the centre of the band where $|\epsilon_k| = 0$. Basically, (14) and (15) get multiplied by somewhat k dependent functions, which may in the long run lead to rather large k variation of J, especially since the approximate solution of (14) and (15) neglecting the k variation diverges: for the isotropic case, for instance

$$\frac{dJ}{\rho J^2} = \frac{dE_c}{E_c - \omega - \Delta}$$

$$\frac{1}{\rho J_0} - \frac{1}{\rho J} \simeq \ln \left(\frac{E_c^0}{E_c - \omega - \Delta} \right)$$

and at some $\omega < -\Delta$ (which, presumably, is the binding energy of the ground state) given by

$$\omega_0 \simeq -\Delta(0) - E_c^0 \exp(-1/\rho J_0) = -\Delta(0) - E_K \tag{17}$$

$\rho J \to \infty$. Near this point

$$\frac{1}{\rho J} = \ln \frac{E_c - \omega - \Delta}{E_K}. \tag{18}$$

While this state of affairs is highly satisfactory from the point of view of finding the binding energy, it does not leave us happy about being able to define the properties of the low states satisfactorily. Continuing ω beyond the pole leads to great complications, and it is more satisfactory to abandon the scaling procedure at some intermediate stage at which $J\rho$ is fairly large at the Fermi surface but not infinite, and to treat the problem the other way round: as a perturbation theory in $1/J\rho$. It will be seen, however, that the complication of (16) is such that it is not easy to define precisely the exact relationship between $J\rho$ and E_c when $J\rho$ is fairly large, just as in the original method cutoff shape dependence left us uncertain as to precise numerical results.

The solution of this strong coupling case is, as in the previous method, complicated without being particularly edifying. It is our impression that the solution in the other method can be given more rigorous limits, and that therefore it is not particularly urgent

to carry it out in detail in the present method, so we will defer it for later publication. The essential nature of it is to define a state ϕ_0 which is an equal linear combination of all k, and couple this in a singlet to S. The coupling of ϕ_0 to free electron states is then a small perturbation of order $1/J\rho$.

The method we have described here looks at first sight like a variant on Suhl's method; (Suhl 1965); in particular, the algebra of equation (10) is identical to some of his manipulations. The physical nature of the method and the results, however, are completely different. We use the formalism *without essential approximation* to scale one problem onto another, rather than making the single particle intermediate state approximation; and we stop short of accepting singularities in our scattering matrix, instead using the method only to scale through an inversion of the coupling parameter from weak to strong. The essential nature of the difficulties of the Kondo problem is thus made clear: one is trapped between a region with all the complications of a true phase transition, and another where the perturbation theory must be done in the inverse of the obvious coupling parameter.

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