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ARE THE SCALING LAWS FOR THE KONDO PROBLEM EXACT?

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ABSTRACT

Anderson's pedestrian way of deriving scaling laws for the Kondo problem, known as "a poor man's derivation", is analysed. It is shown that these scaling equations contain only the first term of a series expansion in powers of the coupling constants. We have constructed a new formulation of the scaling idea to consider higher order terms. The scaling laws obtained in the approximation next to that of the "poor man's derivation" indicate that for low energies the effective coupling tends to a finite value of the order of unity instead of going to infinity, though no final conclusion can be drawn from these scaling laws as this result may be altered if further terms, too, are considered.

РЕЗЮМЕ

Исследуется метод вывода формул законов подобия в эффекте Кондо, данный Андерсоном. Показывается, что полученные Андерсоном законы подобия содержат только первый член разложения по степеням константы связи. Дается новая формулировка идеи подобия, позволяющая учет членов высшего порядка. Законы подобия, полученные в приближении следующем по отношению приближении Андерсона указывают на то, что эффективная константа связи стремится к значению порядка единицы и не к бесконечности, однако нельзя делать окончательный вывод о значении эффективной константы связи на основе полученных нами соотношений, потому что члены более высокого порядка могут изменять наш результат.

KIVONAT

Andersonnak a Kondo-probléma skálatörvényeire adott egyszerü levezetését vizsgáljuk. Megmutatjuk, hogy az általa kapott skálatörvények csak egy, a csatolási állandó hatványai szerint haladó sor első tagját tartalmazzák. A skálázás uj megfogalmazását adjuk, mely lehetővé teszi a magasabb rendü tagok figyelembevételét is. A legegyszerübb közelitésen tuli következő közelitő lépésben az adódik, hogy kis energiáknál az effektiv csatolási állandó egységnyi nagyságrendü lesz és nem tart végtelenhez. Végső következtetést azonban nem lehet levonni, mert a magasabb rendü tagok megváltoztathatják ezt az eredményt.

1. INTRODUCTION

In the development of the theory of the Kondo effect the recent works of Anderson and his co-workers /Anderson and Yuval 1969, Yuval and Anderson 1970, Anderson et al 1970, Anderson and Yuval 1971/ opened up a new field. Anderson and Yuval have shown that the Kondo problem is equivalent to the thermodynamics of a classical one-dimensional Coulomb gas or to that of a one-dimensional Ising problem with inverse-square interaction. By making use of this equivalence, Anderson et al /1970/ were able to derive scaling laws relating the equivalent anisotropic Kondo problems. Scaling was achieved by making a time-scale transformation in the expression of the thermodynamic potential. In the following this scaling will be referred to as thermodynamic scaling. Similar relations were later obtained by Anderson /1970/ in a much simpler way. He considered the scattering matrix T for energies near the Fermi energy and eliminated the contribution of the scattering processes in which in the intermediate state the energy of at least one electron is near the cut-off by introducing an effective coupling. This scaling procedure /it will be referred to as dynamical scaling in the following/, which was claimed to be exact in some sense, led to the conclusion that this effective or re-normalized coupling increases to infinity when the cut-off comes down to the Fermi energy. A priori there is no reason that thermodynamical and dynamical scaling yield the same scaling laws.

Independently from Anderson's paper and from each other, Abrikosov and Migdal /1970/ as well as Fowler and Zawadowski /1971/ applied the re-normalization group technique, well known from quantum field theory, to the Kondo problem. They also introduced effective /"invariant"/ couplings and derived scaling laws for them, though, disregarding the simplest approxima-tion, it has been done for the isotropic Kondo Hamiltonian only. The effective coupling introduced in this way is either energy dependent for fixed cut-off or cut-off dependent for fixed energy taken at the Fermi energy. In the

latter case one expects a one to one correspondence between Anderson's simple approach and these more sophisticated ones. However, the renormalization group method yields an invariant coupling having no singularity, in contrast to Anderson's result. This conclusion is drawn by determining the smallest zero of the infinitesimal generator which has been calculated up to the third order term. Thus by determining further terms it might happen that the exact expression has no zero, which means that the coupling tends to infinity. Further discussion can be found in the papers by Fowler /1972/, Anderson /1973/ and Zawadowski /1973/.

Recently, Wilson /1973/ has calculated the effective coupling by scaling the ground state energy of the Kondo system. His computer calculation indicates that the effective coupling goes to infinity. The problem whether the coupling remains finite or not cannot be resolved in the framework of the dynamical renormalization group and thus it is beyond the scope of the present paper.

In the present paper Anderson's simple derivation of scaling laws is reexamined. It is shown in Sec. 2 that the relations obtained by him are, in fact, the first terms of an expansion in powers of the coupling constant. The problem is reformulated in Sec. 3, where, instead of the usual matrix elements of the T matrix, new matrix elements are introduced in such a way that the proper normalization of the initial and final state wave functions is also considered. The scaling laws are derived in Sec. 4 by using the idea that the change of these matrix elements due to the change of the cut-off energy has to be compensated by a simultaneous variation of the coupling. It is shown in Sec. 5 that, at least up to a given order, these new scaling laws do not result in divergent effective coupling, in agreement with the renormalization group method calculations. The different scaling methods are compared in Sec. 6, where some questions left open in the present derivation of scaling laws are also discussed.

2. ANDERSON'S PEDESTRIAN WAY OF DERIVING SCALING LAWS

The idea used by Anderson to derive the scaling laws for the Kondo problem in a simple manner, was to eliminate the effect of the boundary region of the conduction band /formally changing the cut-off energy/ by introducing a new set of the coupling parameters, called effective couplings. The main steps of this calculation are repeated here to point out the assumptions.

The scattering matrix T obeys the following relation

$$T(\omega) = V + V\,G_0(\omega)\,T(\omega) \quad , \qquad /2.1/$$

where

$$V = \sum_{\substack{k,k' \\ \alpha,\beta}} \left\{ \frac{J_\pm}{2}\left(S^+ s^-_{\alpha\beta} + S^- s^+_{\alpha\beta}\right) + J_z\, S^z\, s^z_{\alpha\beta} \right\} c^+_{k'\alpha}\, c_{k\beta} \qquad /2.2/$$

is the anisotropic Kondo interaction, S is the impurity spin operator, $s_{\alpha\beta}$ is a $s = 1/2$ spin matrix, $c^+_{k\alpha}$ /$c_{k\alpha}$/ is the conduction-electron creation /annihilation/ operator, $J_\pm$ and J_z are the bare coupling constants. Furthermore the Green function and the free Hamiltonian are

$$G_0(\omega) = \left(\omega - H_0\right)^{-1} \quad , \qquad /2.3/$$

$$H_0 = \sum_{k,\alpha} \varepsilon_k\, c^+_{k\alpha}\, c_{k\alpha} \quad , \qquad /2.4/$$

respectively, with ε_k denoting the conduction-electron energy. The interaction V is restricted to an energy range symmetric to the Fermi energy and is limited by cut-offs at $\pm E_c$, the zero of the energy scale being taken at the Fermi energy. Within this energy range the density of conduction-electron states ρ is supposed to be constant.

By introducing a projection operator P which projects onto states containing at least one electron in the energy range /$E_c - \Delta E$, E_c/ or at least one hole in the range /$-E_c$, $-E_c + \Delta E$/, the scattering matrix can identically be decomposed as

$$T = V + V(1-P)\,G_0\,T + V\,P\,G_0\,T \quad . \qquad /2.5/$$

Considering the effect of the projection operator as a small quantity, the iteration of this equation gives in the first step

$$T = \{V + V\,P\,G_0\,V\}$$
$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad /2.6/$$
$$+ \{V + V\,P\,G_0\,V\}\,(1-P)\,G_0\,T + V\,P\,G_0\,V\,P\,G_0\,T \quad .$$

Going to higher and higher orders in the iteration, we can write

$$T = \{V + VPG_oV + VPG_oVPG_oV + \ldots\}$$

$$+ \{V + VPG_oV + VPG_oVPG_oV + \ldots\}(1-P)G_oT$$

$$+ VPG_oVPG_oV\ldots PG_oT \qquad\qquad /2.7/$$

In the n-th step of iteration the last term of eq. /2.7/,

$$\Delta T = VPG_oVPG_oV\ldots PG_oT \quad , \qquad\qquad /2.8/$$

is proportional to J^{n+2} and can be neglected in any perturbational calcula-
tion. The argument that it is negligible because it is proportional to
$/\Delta E/^{n+1}$, will be seen not to be true.

Taking the limit $n\to\infty$ and multiplying eq. /2.7/ by /1-P/ from the left and
from the right, this equation takes the form

$$T' = V' + V' \, G_o \, T' \quad , \qquad\qquad /2.9/$$

where

$$T' = (1-P) \, T(1-P) \quad , \qquad\qquad /2.10/$$

and

$$V' = (1-P)\{V + VPG_oV + VPG_oVPG_oV + \ldots\}(1-P). \qquad /2.11/$$

A comparison of eq. /2.9/ with eq. /2.1/ gives at once that for such scatter-
ing processes, in which in both the initial and final states the electron
energies are farther from the cut-off than ΔE, the original problem with
interaction V and cut-off E_c is equivalent to a new problem with cut-off
at $E_c-\Delta E$ and interaction V' given by eq. /2.11/.

Looking at the matrix elements of the scattering matrix between
one-particle excited states, in some approximation this new interaction may
have a spin structure similar to that of the original interaction. In this
way effective coupling constants, J'_z and $J'_\pm$ can be defined. In the anisotropic
case this can be done for S = 1/2 only. For general spin the spin products do
not simplify to the form of eq. /2.2/. Moreover these effective couplings
depend generally on ω and on the energies of the incoming and outgoing electrons
as well. For the sake of simplicity these electron energies ε_k and $\varepsilon_{k'}$ will be
taken at the Fermi energy.

Using this procedure the original problem is scaled into a new
equivalent problem, where the effect of those states which are eliminated by
the new cut-off is taken into account by the effective coupling. If the change

of the cut-off, ΔE, is small enough, a differential equation can be derived for the effective coupling, relating the equivalent problems.

For getting this differential equation, $\Delta V = V' - V$ has to be calculated up to terms linear in ΔE. Anderson claimed that the third term in V', $VPG_o VPG_o V$, which contains twice the projection operator P in the intermediate states, is quadratic in ΔE and thus it is negligible. It will be shown, however, that this term does give contribution linear in ΔE.

The contributions to ΔV can be represented very simply by time-ordered diagrams. This is illustrated on the first term of ΔV which has been investigated by Anderson.

$$\Delta V^{(1)} = \sum_{\substack{k_1,k_2 \\ \alpha,\beta}} \left\{ \frac{J_\pm}{2} \left(s^+ s^-_{\alpha\beta} + s^- s^+_{\alpha\beta} \right) + J_z \, s^z \, s^z_{\alpha\beta} \right\} c^+_{k_1,\alpha} c_{k_2\beta}$$

$$/2.12/$$

$$\times P \frac{1}{\omega - H_o} \sum_{\substack{k_3,k_4 \\ \gamma,\delta}} \left\{ \frac{J_\pm}{2} \left(s^+ s^-_{\gamma\delta} + s^- s^+_{\gamma\delta} \right) + J_z \, s^z \, s^z_{\gamma\delta} \right\} c^+_{k_3\gamma} c_{k_4\delta} .$$

Due to the projection operator P an electron is either created by $c^+_{k_3}$ in the energy range $/E_c - \Delta E, E_c/$ or destroyed by c_{k_4} in $/-E_c, -E_c + \Delta E/$.

As we are interested in scattering processes where an electron with momentum k $/\varepsilon_k = 0/$ is scattered into another state with momentum k' $/\varepsilon_{k'} = 0/$ and the rest of the Fermi sea is unchanged, ΔV^1 can be transformed to

$$\Delta V^{(1)} = \sum_{k,\alpha} \sum_{k',\beta} \sum_{k_1,\gamma}^{E_c - \Delta E < \varepsilon_{k_1} < E_c} \frac{1}{\omega - E_c + \varepsilon_k} c^+_{k'\beta} c_{k_1\gamma} c^+_{k_1\gamma} c_{k\alpha}$$

$$\times \left\{ \frac{J^2_\pm}{4} \frac{1}{2} \left(s^+ s^- + s^- s^+ \right) \delta_{\alpha\beta} + \frac{J^2_z}{4} \left(s^z \right)^2 \delta_{\alpha\beta} \right.$$

$$\left. - \frac{J_\pm J_z}{2} \frac{1}{2} \left(s^+ s^-_{\alpha\beta} + s^- s^+_{\alpha\beta} \right) - \frac{J^2_\pm}{2} s^z \, s^z_{\alpha\beta} \right\}$$

$$/2.13/$$

$$+ \sum_{k,\alpha} \sum_{k',\beta} \sum_{k_1,\gamma}^{-E_c < \varepsilon_{k_1} < -E_o + \Delta E} \frac{1}{\omega - E_c - \varepsilon_{k'}} c^+_{k_1\gamma} c_{k\alpha} c^+_{k'\beta} c_{k_1\gamma}$$

$$\times \left\{ \frac{J^2_\pm}{4} \frac{1}{2} \left(s^+ s^- + s^- s^+ \right) \delta_{\alpha\beta} + \frac{J^2_z}{4} \left(s^z \right)^2 \delta_{\alpha\beta} \right.$$

$$\left. + \frac{J_\pm J_z}{2} \frac{1}{2} \left(s^+ s^-_{\alpha\beta} + s^- s^+_{\alpha\beta} \right) + \frac{J^2_\pm}{2} s^z \, s^z_{\alpha\beta} \right\} .$$

The two scattering processes corresponding to these two terms are displayed schematically in Fig. 1. In these time-ordered diagrams the electrons are represented by lines running from left to right, while the holes by lines running from right to left. The electrons or holes which are in the narrow energy range $/E_c - \Delta E, E_c/$ or $/-E_c, -E_c + \Delta E/$, are distinguished by heavy lines.

The integration over k_1 gives simply a factor $\rho \Delta E$. Neglecting the energies of the scattered electrons ε_k and $\varepsilon_{k'}$, compared with E_c, eq. $/2.13/$ yields

$$\Delta V^{(1)} = \Delta V_o + \sum_{\substack{k,k' \\ \alpha,\beta}} \left\{ \frac{\Delta J_\pm}{2} \left(S^+ s^-_{\alpha\beta} + S^- s^+_{\alpha\beta} \right) + \Delta J_z \, S^z \, s^z_{\alpha\beta} \right\} c^+_{k'\beta} \, c_{k\alpha} \quad , \qquad /2.14/$$

with

$$\Delta V_o = \frac{\rho \Delta E}{8} \left(J_z^2 + 2 J_\pm^2 \right) \sum_{k=o}^{k_c} \left(\omega - E_c - |\varepsilon_k| \right)^{-1} \quad , \qquad /2.15/$$

$$\Delta J_\pm = - \frac{\rho \Delta E}{\omega - E_c + \Delta} \, J_\pm \, J_z \quad , \qquad /2.16/$$

$$\Delta J_z = - \frac{\rho \Delta E}{\omega - E_c + \Delta} \, J_\pm^2 \qquad /2.17/$$

ΔV_o gives a shift of the ground state energy and is incorporated into eqs. $/2.16/$ and $/2.17/$ by means of Δ.

The ground state energy shift will not be further investigated here. Writing these relations in differential form we get

$$\frac{dJ_\pm}{dE_c} = - \frac{\rho}{\omega - E_c + \Delta} \, J_\pm \, J_z \quad , \qquad /2.18/$$

$$\frac{dJ_z}{dE_c} = - \frac{\rho}{\omega - E_c + \Delta} \, J_\pm^2 \qquad . \qquad /2.19/$$

If higher-order processes give no contribution, as Anderson suggested, these scaling laws would be exact. Now we will show that this is not the case.

Let us look at the processes in V' which are of third order in $J_\pm$ or J_z. They are represented by the diagrams shown in Fig. 2. In both

intermediate states there is one electron or one hole in the energy range $/E_c - \Delta E, E_c/$ or $/-E_c, -E_c + \Delta E/$. As always the same electron is in this range in both intermediate states, the contribution is proportional to ΔE and not to $/\Delta E/^2$. Similarly there are higher-order processes, too, which yield contribution to ΔV proportional to ΔE, and consequently contribute to the scaling laws. As a matter of fact the scaling laws, as given in eqs. /2.16/ and /2.17/, contain on their right-hand sides only the first terms of a series expansion in powers of the coupling constants.

The contribution of these processes depends on a non-trivial way on the energies ε_k and ε'_k and no scaling law can be derived for the total scattering matrix, only for those of its matrix elements where ε_k and $\varepsilon_{k'}$ are small. Moreover, in an attempt to get scaling laws in higher orders by the abovementioned method, another difficulty arises. Namely the T matrix describes also such scattering processes in which more than one electron is scattered from the initial to the final state. These processes cannot be scaled into the original problem, where only one-electron scattering processes exist.

For these reasons we will reformulate Anderson's treatment to make it extensible to higher orders.

3. REFORMULATION OF THE PROBLEM

From the above discussion it follows that instead of the total scattering matrix its matrix elements

$$T_{fi} = <f|T|i>$$
/3.1/

should be considered, where the initial and final states contain one excited electron.

$$|i> = c^+_{k\alpha}|0> \quad , \quad |f> = c^+_{k'\beta}|0> \quad ,$$
/3.2/

and $|0>$ is the non-interacting Fermi sea plus an impurity spin. The energies will be taken at the Fermi energy. Instead of rearranging eq. /2.1/ for the scattering matrix we will proceed in a different way to define an effective coupling. Let us change the cut-off E_c by ΔE and simultaneously the coupling constants $J_\pm$ and J_z by $\Delta J_\pm$ and ΔJ_z, respectively. We require that the matrix element T_{fi} be unchanged under this transformation, i.e. the following relation must hold

$$T_{fi}\left(E_c, J_\pm, J_z\right) = T_{fi}\left(E_c - \Delta E, J_\pm + \Delta J_\pm, J_z + \Delta J_z\right)$$
/3.3/

For small changes of the parameters first-order expansion gives

$$- \frac{\partial T_{fi}}{\partial E_c} \Delta E + \frac{\partial T_{fi}}{\partial J_\pm} \Delta J_\pm + \frac{\partial T_{fi}}{\partial J_z} \Delta J_z = 0 \quad . \tag{/3.4/}$$

By calculating the derivatives to a given order and collecting the terms containing $s^z s^z$ and $1/2 \left(s^+ s^- + s^- s^+ \right)$, two equations are obtained for the variation of the two coupling constants.

This is not a formal transcription of the original formulation: more processes are considered in this way than in the earlier version, as it will be seen in the next section. These additional processes are due to self-energy corrections for the impurity spin and are related to the re-normalization of the initial and final states. This indicates that the change of the norm of the wave function has to be included as well into this consideration. Therefore instead of /3.1/ the following matrix element will be investigated

$$T'_{fi} = \frac{\langle f | V + V \frac{1}{\omega - H_o} T | i \rangle}{\sqrt{\langle f | 1 + \frac{1}{\omega - H_o} T | f \rangle \langle i | 1 + \frac{1}{\omega - H_o} T | i \rangle}} \tag{/3.5/}$$

where T is the usual T matrix. The invariance of this quantity will be required, thus the scaling laws will be obtained from

$$- \frac{\partial T'_{fi}}{\partial E_c} \Delta E + \frac{\partial T'_{fi}}{\partial J_\pm} \Delta J_\pm + \frac{\partial T'_{fi}}{\partial J_z} \Delta J_z = 0 \quad . \tag{/3.6/}$$

A discussion of this choice will be given later.

4. EVALUATION OF THE T MATRIX

Up to second order in the coupling constant T'_{fi} is obtained in a straightforward manner,

$$T'^{(2)}_{fi} = T^{(2)}_{fi} = \frac{J_\pm}{2} \left(s^+ s^- + s^- s^+ \right) + J_z s^z s^z$$

$$- \left\{ \frac{J_\pm J_z}{2} \left(s^+ s^- + s^- s^+ \right) + J_\pm^2 s^z s^z \right\} \rho \ln \frac{\omega}{E_c} \quad . \tag{/4.1/}$$

In this order the wave function is not renormalized. Inserting /4.1/ into /3.4/ the same scaling laws are obtained as by Anderson's method /see eq. /2.18/ and /2.19//.

The third-order correction to T'_{fi} will not be given here in detail. For the derivative of T'_{fi} with respect to the coupling constants it is sufficient to take the second-order expression of T'_{fi} as from the lowest-order scaling it is known that ΔJ is proportional to J^2. As for the derivative with respect to the cut-off E_c, it can be calculated directly using the diagrammatic method of Sec. 2. In addition to the graphs of Fig. 2 there are 12 more third-order scattering processes depicted in Fig. 3 which are proportional to ΔE.

The processes corresponding to the first eight graphs in Fig. 3 can be accounted for in Anderson's way of introducing the new effective interaction. The last four processes, however, which correspond to the polarization of the impurity spin state and thus describe the renormalization of the initial and final states, can be taken into account in this new formulation only. Half of the contribution of these diagrams is cancelled by the denominator of /3.5/. These processes and this cancellation will turn out to be very important.

Neglecting the ground state energy shift, the corresponding scaling law will not be considered here, we get in the limit $\omega \ll E_c$

$$\Delta T'_{fi} = \frac{\rho}{E_c}\left\{ J_\pm^2\, s^z\, s^z + J_\pm J_z\, \frac{1}{2}\left(s^+ s^- + s^- s^+\right)\right\}\Delta E$$

$$- \frac{\rho^2}{E_c^2}\left\{ \frac{J_\pm^2 J_z}{2}\, s^z\, s^z + \left(\frac{J_\pm J_z^2}{4} + \frac{J_\pm^3}{4}\right)\frac{1}{2}\left(s^+ s^- + s^- s^+\right)\right\}\Delta E$$

$$- \frac{\rho^2}{E_c^2} \ln\frac{\omega}{E_c}\left\{ 2J_\pm^2 J_z\, s^z\, s^z + \left(J_\pm J_z^2 + J_\pm^3\right)\frac{1}{2}\left(s^+ s^- + s^- s^+\right)\right\}\Delta E + \dots$$

$$/4.2/$$

Inserting /4.2/ and the derivative of /4.1/ with respect to J_+ and J_z into /3.6/ and collecting the terms proportional to $\frac{1}{2}\left(s^+ s^- + s^- s^+\right)$ and $s^z s^z$, respectively, the following two equations are obtained

$$- \frac{\rho}{E_c} J_\pm J_z\, \Delta E + \frac{\rho^2}{E_c^2}\left(\frac{J_\pm J_z^2}{4} + \frac{J_\pm^3}{4}\right)\Delta E$$

$$+ \frac{\rho^2}{E_c^2} \ln\frac{\omega}{E_c}\left(J_\pm J_z^2 + J_\pm^3\right)\Delta E + \Delta J_\pm \qquad /4.3/$$

$$- \rho \ln\frac{\omega}{E_c} J_z\, \Delta J_\pm - \rho \ln\frac{\omega}{E_c} J_\pm\, \Delta J_z = 0 \quad ,$$

$$- \frac{\rho}{E_c} J_{\pm}^2 \, \Delta E + \frac{\rho^2}{E_c} \frac{J_{\pm}^2 J_z}{2} \Delta E + \frac{\rho^2}{E_c} \ln \frac{\omega}{E_c} 2J_{\pm}^2 \, J_z \, \Delta E$$

$$+ \Delta J_z - \rho \ln \frac{\omega}{E_c} 2J_{\pm} \, \Delta J_{\pm} = 0 \quad . \qquad\qquad /4.4/$$

The solution of these equations up to third order is

$$\Delta J_{\pm} = \frac{\rho}{E_c} \left\{ J_{\pm} J_z - \frac{1}{4} \left(J_{\pm} J_z^2 + J_{\pm}^3 \right) \rho \right\} \Delta E \quad , \qquad\qquad /4.5/$$

$$\Delta J_z = \frac{\rho}{E_c} \left\{ J_{\pm}^2 - \frac{1}{2} J_{\pm}^2 \, J_z \, \rho \right\} \Delta E \quad . \qquad\qquad /4.6/$$

In differential form eqs. /4.5/ and /4.6/ read

$$\frac{dJ_{\pm}}{dE_c} = \frac{\rho}{E_c} \left\{ J_{\pm} J_z - \frac{1}{4} \left(J_{\pm} J_z^2 + J_{\pm}^3 \right) \rho \right\} \quad , \qquad\qquad /4.7/$$

$$\frac{dJ_z}{dE_c} = \frac{\rho}{E_o} \left\{ J_{\pm}^2 - \frac{1}{2} J_{\pm}^2 \, J_z \, \rho \right\} \quad . \qquad\qquad /4.8/$$

In these equations we have got to the first corrections to the scaling laws
of /2.18/ and /2.19/.

5. DISCUSSION OF THE SCALING LAWS

The usefulness of the scaling laws is to establish connection
between anisotropic Kondo-type interactions with different coupling constants.
In Anderson's approximation the equivalent Kondo problems form hyperbolas in
the $/J_{\pm}$, $J_z/$ plane. From this it was calculated that for $J_z < 0$ and $J_{\pm} \leq |J_z|$
the problem is scaled into a soluble problem with $J_{\pm} = 0$. In other cases,
especially for the isotropic Kondo problem with $J_{\pm} = J_z > 0$, the gradual
change of the cut-off to lower values led to an increase of the effective
coupling to infinity. In Anderson's view, however, this does not mean that
the problem is unsolvable for $J_z > 0$. There is a value of J_z /$J_z \rho \approx 2/\pi$/, where
the problem becomes trivially soluble. This is the Toulouse limit /Toulouse
1969, Anderson et al. 1970/. The Kondo problem is thus scaled into this limit.

The new scaling laws of /4.7/ and /4.8/ change the situation
drastically. The equivalent problems in this approximation /the trajectories
of this system of differential equations/ can be seen in Fig. 4. The arrows

on the trajectories show the trend of scaling when the cut-off decreases. There exists an isolated singular point in the $/J_+ , J_z/$ plane at $J_+\rho = = J_z\rho = 2$ and all the possible anisotropic Kondo problems scale into this point, except for the region $J_z < 0$ and $J_+ \leq |J_z|$. This region, as in Anderson's approximation, scales to the solvable $J_+ = 0$ case.

The scaling laws of /4.7/ and /4.8/ are of course not valid for large $J_+\rho$ and $J_z\rho$, as the higher-order corrections on the right-hand sides of these equations have been neglected. Therefore approaching the isolated singular point this approximation breaks down. In general we can only claim that the scaling equations may have the form

$$\frac{dJ_\pm}{dE_c} = \frac{\rho}{E_c} \; f\left(J_\pm , J_z\right) , \qquad\qquad /5.1/$$

$$\frac{dJ_z}{dE_c} = \frac{\rho}{E_c} \; g\left(J_\pm , J_z\right) , \qquad\qquad /5.2/$$

where f and g are unknown functions and their power series starts as /4.7/ and /4.8/. Because isotropic case is always scaled into isotropic one, $f(J,J) = g(J,J)$. The question remains whether the function $f(J,J)$ has a simple zero, as it has in our approximation, or not. If it has at least one simple zero, this point will be an isolated singular point in the (J_+ , J_z) plane and it will give an upper limit for the effective coupling. If, however, $f(J,J)$ has no zero, the effective coupling is not bounded and Anderson's reasoning is valid. This question cannot be answered in the framework of the present method, because the exact expressions of the functions f and g are not known.

Supposing that the infinitesimal generator has a zero, there are still two possibilities depending whether the upper limit for the effective coupling is smaller or larger than the value corresponding to the Toulouse limit. If it is larger, the weak coupling Kondo problem is then scaled into the Toulouse limit before arriving to the situation corresponding to the isolated singular point and the problem is solvable.

6. COMPARISON WITH OTHER METHODS

In the preceding section we have derived scaling laws relating the equivalent Kondo problems. Following Anderson's method /Anderson 1970/ the effective coupling has been introduced through the requirement that the original problem and the new one, with slightly modified cut-off and coupling

Constants, give the same scattering matrix elements. This procedure yields effective couplings which depend in addition to the original and new cut-offs, on ω and on the electron energies ε_k, ε_k, as well. In the actual calculation these energies have been taken near the Fermi energy and could be neglected compared to the cut-off energy. In the general case, however, this dependence can be important.

In the present paper the imaginary parts contributing to the scattering matrix have been neglected everywhere. They give no contribution to the scaling laws in lowest order. In higher orders, however, they must play an important role and might eventually lead to complex effective couplings, although physically we expect the couplings to remain real.

Another problem of the present derivation is that the scaling laws were obtained not from the usually defined T matrix but from /3.5/, where the change of the norm of the initial and final wave functions has also been taken into consideration. Neglecting this wave function renormalization or using Anderson's original approach, quite different scaling laws would have been obtained in third order. All these problems clearly show the shortcomings of this sort of treatment of the scaling.

The problem of the energy dependence of the effective coupling, the role of the imaginary parts of the T matrix and the problem whether the wave function normalization should be considered or not, can be solved by a consequent application of the renormalization group method only /Bogoliubov and Shirkov 1959/. This technique was used for the Kondo problem by Fowler and Zawadowski /1971/ and by Abrikosov and Migdal /1970/.

In case of the Kondo problem the effective or invariant coupling is introduced in the renormalization group method as the product of the vertex Γ and the normalizing factor of the pseudo-fermion Green function $d = \mathcal{G}/\mathcal{G}_0$.

$$J_{inv} = \Gamma d \ . \qquad\qquad /6.1/$$

The invariance of this quantity under multiplicative renormalization of the Green functions and vertices, which is equivalent to an energy scale transformation, ensures that the properly defined effective coupling can be obtained from /3.4/, provided this invariant combination is used there instead of the usual T matrix. T'_{fi} , as defined in /3.5/, satisfied this invariance requirement. Anderson's approach of regrouping the terms in the scattering matrix corresponds to taking Γ only, while the total T matrix without correcting for the wave function normalization is equivalent to taking Γd^2. The denominator in T'_{fi} cancels the extra factor d and therefore T'_{fi} is invariant under the scale transformation. This confirms the choice of T'_{fi} in eq. /3.6/.

In the renormalization group technique the invariant coupling does not depend on the particular choice of the variables of the vertex. This is not the case here. In the limit, though, when the energies are small compared with the cut-off energy, the same scaling laws are obtained by the present method as from the renormalization group technique.

The role of the imaginary parts is more delicate. Even in the renormalization group method it is not trivial that the invariant coupling is always real. We will show in another paper that at least in a given approximation the imaginary parts cancel out and the invariant coupling is in fact real. This does not solve, however, the problem: what the role of the imaginary parts is in the observable quantities. Their effect is very important if a comparison with experimental results is attempted.

The relation of the present results to the thermodynamic scaling of Anderson et al. /1970/ is not settled. These authors started from the thermodynamic potential which contains the effect of all electrons in an averaged manner. Electrons, whose energy is comparable with the cut-off energy, can give important contribution. Thermodynamic scaling can therefore lead to different scaling laws than dynamical scaling, where only electrons with low energy were taken into account. In fact, the scaling laws obtained by Anderson et al. do not coincide with our result. These scaling laws contain higher order corrections, similarly as in the present paper, though the coefficients may be different as they are different in the third order, in the next step after the "poor man's" result. Because our result agrees with that of the sophisticated renormalization group technique, we are confident that we have got correctly the third-order corrections in dynamical scaling.

The most important problem in the Kondo effect is to decide whether in the dynamical scaling laws the invariant coupling remains finite or tends to infinity as it has been suggested by Anderson and Wilson /1973/ in the thermodynamical scaling. The relationship between the dynamical and thermodynamical scalings is also not settled, actually they are different in the third order. These problems have to be solved to have a physical understanding of the Kondo problem.

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FIGURE CAPTIONS

Fig. 1   Second-order scattering processes in time-ordered diagrams.
          The heavy lines represent electrons or holes the energy of which
          is in the range $/E_c-\Delta E$, $E_c/$ or $/-E_c$, $-E_c+\Delta E/$.

Fig. 2   Third-order processes contributing to ΔV.

Fig. 3   Third-order processes contributing to ΔT.

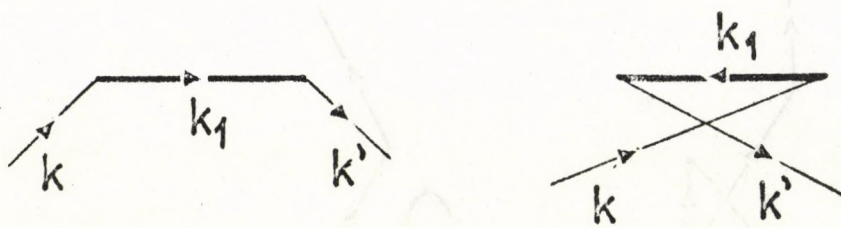Fig. 4   Scaling curves of the anisotropic Kondo problem in third-order
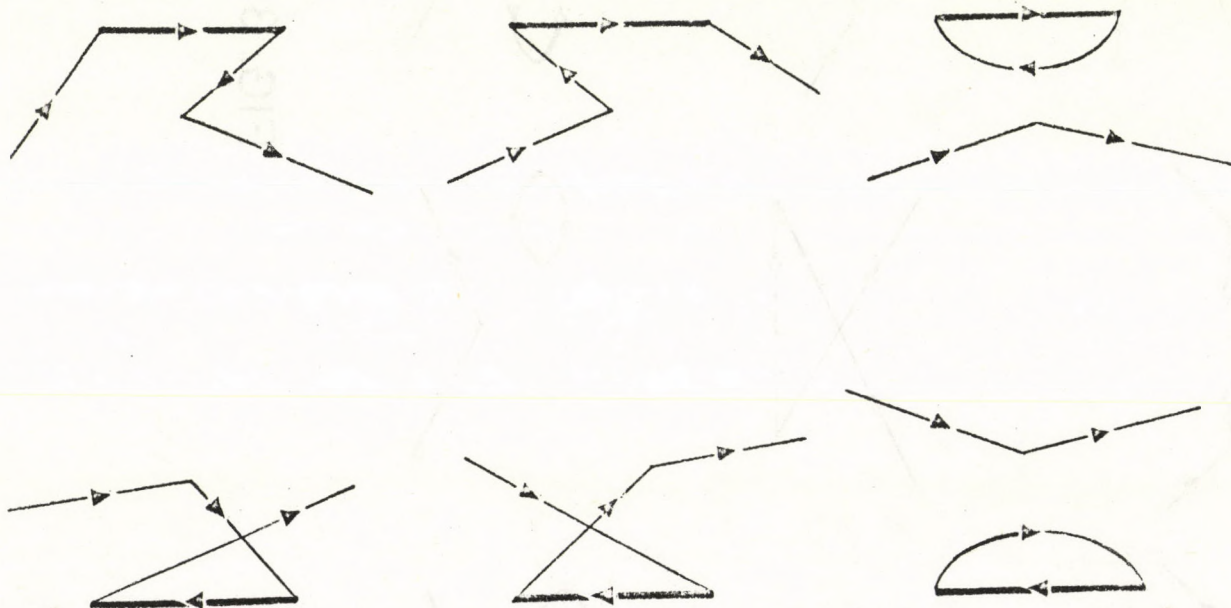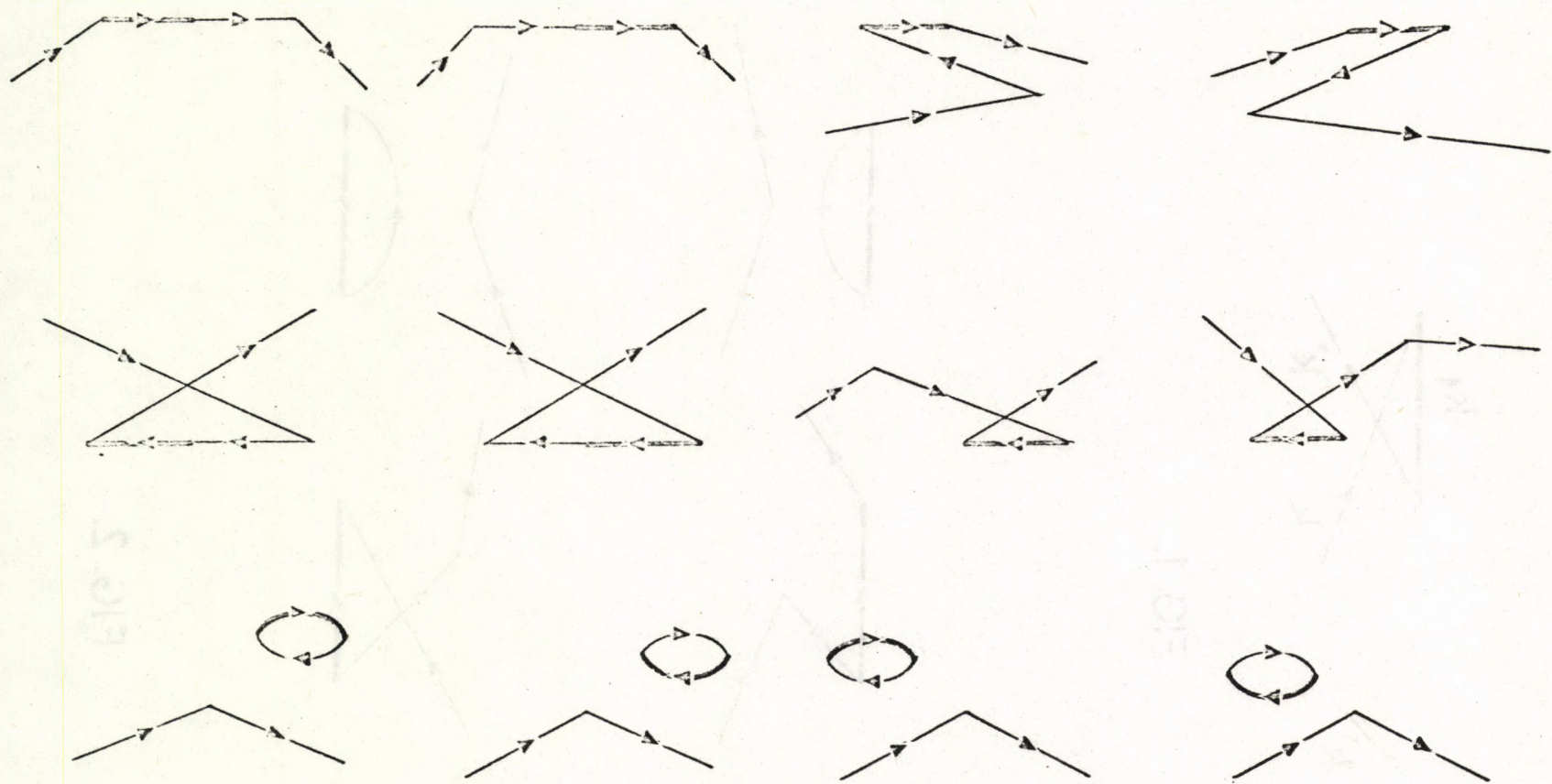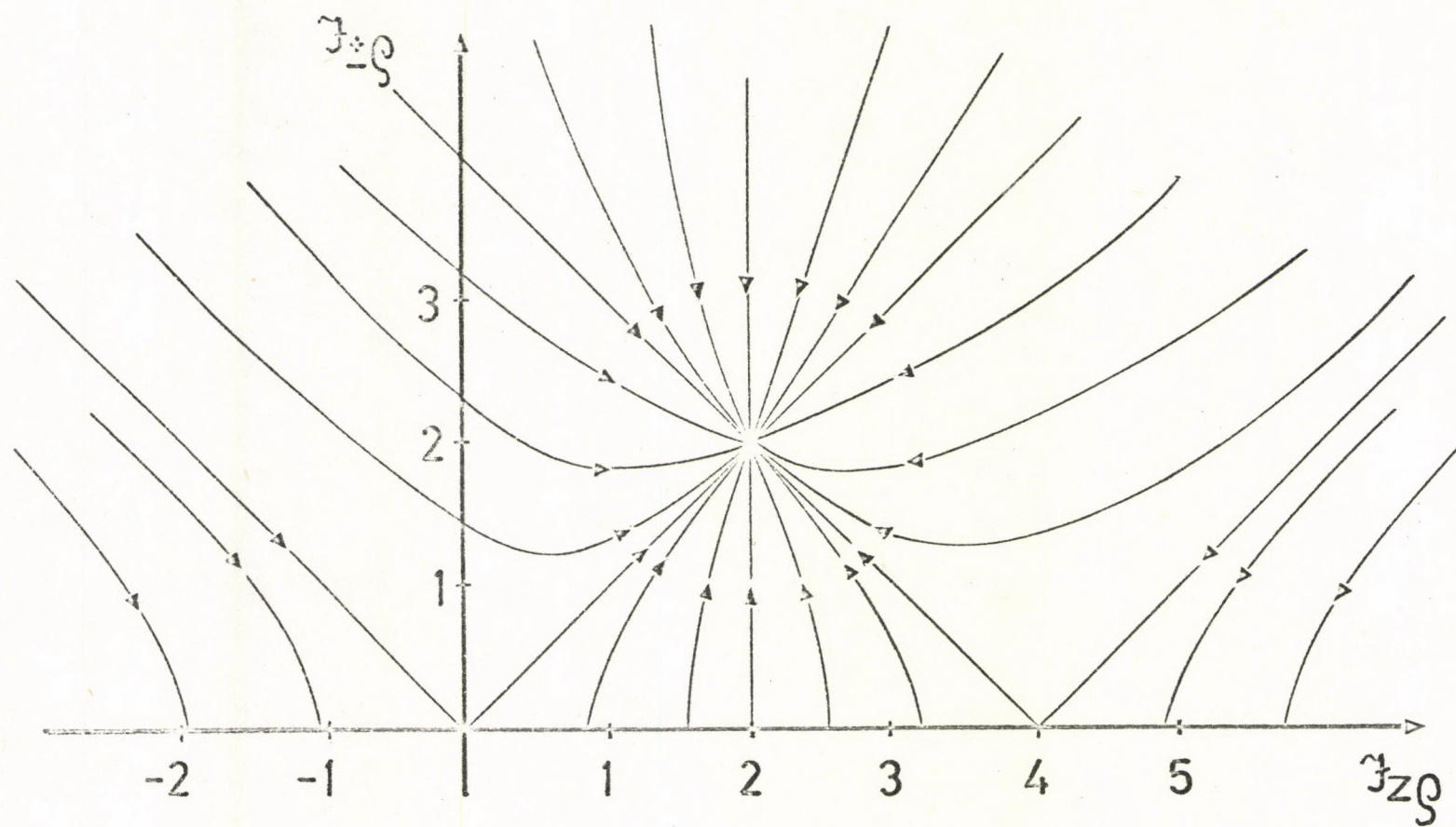   scaling.

FIG. 1.

FIG. 2.

FIG. 3.

FIG. 4.

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