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RENORMALIZATION AND SCALING IN THE X-RAY ABSORPTION AND KONDO PROBLEMS

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ABSTRACT

The renormalization group method is extended in case of logarithmic problems to include the imaginary parts of Green's functions and vertices, which have been neglected in the earlier versions of the theory. The relationship between multiplicative renormalization and scaling of the characteristic energy is demonstrated and is used to investigate the x-ray absorption and Kondo problems. The properly defined invariant couplings depend on a single variable, the scaling energy, and are real, as expected physically. The scaling laws are rederived on this more rigorous basis. It is shown that the imaginary parts of the Green's functions and vertices give no contribution to the scaling laws. In particular in the Kondo problem the scaling laws obtained earlier remain intact, indicating that in this improved theory as well the potential scattering is not renormalized and is not coupled to the exchange scattering.

РЕЗЮМЕ

Дается такое обобщение метода группы ренормировок, которые в случае логарифмических задач позволяет учитывать мнимую часть функции Грина и вершинных функций, которая не была раньше учтена. Показывается взаимосвязь между методом мультипликативной перенормировки и скэлингом характеристикой энергии. Взаимосвязь указанных двух методов используется в исследованиях по поглощению рентгеновских лучей и эффекту Кондо. Правильно определенная эффективная константа связи зависит только от одной переменной, от энергии скэлинга и является вещественной как ожидается на основе физических соображений. Дается строгий вывод законов подобия. Показано, что мнимая часть функций Грина и вершинных функций не дает вклада в законы подобия. В случае исследования по эффекту Кондо соответствующие законы подобия не изменяются в результате учета мнимых частей, что указывает на то,что в этой улучшенной теории потенциальное рассеяние не ренормируется и оно не связано с обменным взаимодействием.

KIVONAT

Logaritmikus problémák esetén kiterjesztettük a renormálási csoportmódszert a Green-függvények és vertexek imaginárius részének figyelembevételére, mert ezt a korábbi elméletek elhagyták. Megmutatjuk, hogy a multiplikativ renormálás és a karakterisztikus energia skálázása egyenértékű, s ezt felhasználjuk a röntgenabszorpció és a Kondo-probléma vizsgálatára. A helyesen definiált invariáns csatolás csak egy változótól, a skálaenergiától függ, és valós, ahogyan ez fizikailag várható. Levezetjük a skálatörvényeket ezen az uj módon. Megmutatjuk, hogy a Green-függvények és vertexek imaginárius részei nem adnak járulékot a skálatörvényekhez. A Kondo-probléma esetén a korábban kapott skálatörvényeket kapjuk változatlanul. Ebben a javitott elméletben sem renormálódik a potenciálszórás és nem csatolódik az s-d szórással.

I. Introduction

Multiplicative renormalization and the renormalization group have been first introduced in quantum electrodynamics[1,2] where the divergent charge and mass corrections have been renormalized to get the observable finite charge and mass. Since then this method has been widely used in quantum field theory. The same renormalization group approach has been applied in solid state physics by Abrikosov and Migdal[3] as well as by Fowler and Zawadowski[4] to investigate infrared divergences in the Kondo problem and by Zawadowski[5] in the x-ray absorption problem[6,7]. By analogy with quantum electrodynamics an "invariant charge" was introduced, the energy /or temperature/ dependence of which characterizes the behaviour of the system. For the Kondo problem this invariant charge is a smooth function of its variable without any singularity at the Kondo energy E_K /or Kondo temperature T_K/, tending to a finite value at $E=0$ /or $T=0$/. As a consequence the low energy or low temperature /$T \ll T_K$/ behaviour of the physical quantities is given by power laws.

Another recent attempt to derive scaling laws for the Kondo problem was made by Anderson et al.[8] in a sophisticated manner and later by Anderson[9] in a pedestrian way. In the former case[8] the Kondo problem was formulated as a succession of spin flips. The system's readjustment after each spin flip can be described analogously to the x-ray absorption process[6]. By making a scale transformation of the characteristic time elapsing between successive spin flips Anderson et al. have found scaling laws relating the equivalent anisotropic Kondo models. These scaling laws have been rederived by Anderson by scaling the characteristic energy /cut-off energy/ of the Kondo problem.

The two abovementioned approaches yielded different scaling laws and led to different conclusions concerning the equivalent Kondo problems. Zawadowski and the present author[10] have shown that an extension of Anderson's simple scaling idea to higher orders gives the same scaling laws as the renormalization group method. Inspite of this there is still a disagreement in the interpretation. The difficulty of the Kondo problem is that the invariant coupling tends to infinity or to a value of the order of unity, while the scaling laws are known for small values of the invariant coupling only. We are not going to discuss these two possibilities, a review of our present understanding of the Kondo problem can be found in the papers by Anderson[11], Fowler[12] and Zawadowski[13]. Here we concentrate our attention to other aspects of renormalization and scaling.

The proper definition of the "invariant charge" or invariant coupling is not settled in either of the above mentioned approaches. Though the invariant charge is determined via complex Green's functions and vertices, it is expected to be real to have physically reasonable meaning. Hitherto either the imaginary parts have been neglected, or the invariant coupling has been determined in a particular range of the variables where no imaginary part exists. The aim of the present paper is to give an unambiguous definition of the invariant coupling for logarithmic problems and to derive the scaling laws by taking into account the imaginary parts of the Green's functions and vertices.

In Sec. II the relationship between multiplicative renormalization of the Green's function and vertices and scaling of the characteristic energy is discussed for logarithmic problems. This relationship allows us to define an invariant coupling which in special cases coincides with the usual definition. The invariant couplings are determined in Sec. III and IV for the x-ray absorption problem and the Kondo problem, respectively. They are in fact real as it is demonstrated on these two examples and depend on the scaling energy only. The scaling laws obtained in this way coincide with those obtained by Fowler and Zawadowski, indicating that the imaginary parts have no bearing on the scaling laws. By investigating the T matrix of the

Kondo problem it is shown that even if the invariant coupling were known, all the skeleton graphs should have to be considered to get reliable expressions for the physical quantities. The discussion of the results is given in Sec. V. The anisotropic Kondo model is investigated in an Appendix. Here again the imaginary parts of the Green's functions and vertices leave intact the scaling laws derived earlier by Sólyom and Zawadowski.

II. Relationship between multiplicative renormalization and scaling in logarithmic problems

Multiplicative renormalization is a simple transformation procedure in which the Green's functions, vertices and coupling constants are multiplied by real, frequency independent factors, z_i. The requirement that the Dyson equation be satisfied by the original and transformed quantities as well, gives a relation between these factors. The arbitrariness in the choice of the multiplicative factors can be incorporated into the Green's functions and vertices themselves by introducing an extra variable λ, the variation of which is equivalent to different choices of the z_i's. Usually the physical solution corresponds to a particular choice of the dummy variable λ, or to a particular set of the renormalizing factors.

This classical formulation of multiplicative renormalization was used by Fowler and Zawadowski[4] to get scaling laws for the Kondo problem. The imaginary part of the Green's function and vertices has been neglected, however, in this treatment. The same applies to the work of Abrikosov and Migdal[3]. On the other hand the introduction of the variable λ is not unambiguous. These two problems show the necessity to give a proper definition of the invariant coupling. This will be done here for logarithmic problems.

From Anderson's approach[9] to the scaling laws for the Kondo problem we can infer that the cut-off energy can serve as a natural scaling parameter. On this ground it is suggested here that, at least for logarithmic problems, multiplicative renormalization can be achieved without introducing the dummy variable λ.

Let us take for illustration a system of interacting electrons with bare coupling constant g. The total Green's function and the total vertex is written in the form

$$G = G_0 d \; , \qquad /2.1/$$

and

$$\Gamma = g \tilde{\Gamma} \; . \qquad /2.2/$$

For simplicity the momentum variables are fixed at the Fermi momentum and only the frequency variables are retained. If the interaction is cut off at an energy ω_0, the Green's function and vertices depend, as a rule, on the relative energies ω/ω_c.

Multiplicative renormalization is formulated usually as the transformation

$$G \to z_1 G \quad \text{or} \quad d \to z_1 d , \qquad /2.3/$$

$$\tilde{\Gamma} \to z_2^{-1} \tilde{\Gamma} , \qquad /2.4/$$

$$g \to z_1^{-2} z_2 g , \qquad /2.5/$$

where z_1 is independent of the frequency variable ω. In logarithmic problems we can try to avoid the introduction of an extra variable and to achieve this multiplicative renormalization by varying the cut-off ω_c. Performing a simultaneous change of the cut-off ω_o to ω_o' and the bare coupling constant g to g', g' is determined from the requirement that

$$d\left(\frac{\omega}{\omega_o'}, g'\right) = z_1\left(\frac{\omega_o'}{\omega_c}, g\right) d\left(\frac{\omega}{\omega_o}, g\right), \qquad /2.6/$$

$$\tilde{\Gamma}\left(\frac{\omega_1}{\omega_c'}; \frac{\omega_2}{\omega_c'}, \frac{\omega_3}{\omega_o'}, \frac{\omega_4}{\omega_o'}, g'\right) = z_2^{-1}\left(\frac{\omega_o'}{\omega_o}, g\right) \tilde{\Gamma}\left(\frac{\omega_1}{\omega_c}, \frac{\omega_2}{\omega_o}, \frac{\omega_3}{\omega_c}, \frac{\omega_4}{\omega_c}, g\right), \qquad /2.7/$$

$$g' = z_1^{-2}\left(\frac{\omega_o'}{\omega_o}, g\right) z_2\left(\frac{\omega_o'}{\omega_o}, g\right) g . \qquad /2.8/$$

Whether this transformation to the primed variables can be done with real z_i is not a priori true for any problem. Our guess is that these relations can be satisfied for logarithmic problems. Such a treatment was already presented by Menyhárd and the present author[14,15] for one-dimensional metallic systems, where the cut-off energy is in fact a good scaling parameter. We have shown that, at least up to third order in the coupling constants, the relations analogous to eqs. /2.6/-/2.8/ can be satisfied with real z_i which are independent of the frequency variables. It will be demonstrated here that the same holds for the x-ray absorption problem as well as for the Kondo problem.

If relations /2.6/-/2.8/ are obeyed, the cut-off dependent g', the self-consistent solution of the equation

$$g' = g \, \frac{\tilde{\Gamma}\left(\frac{\omega_1}{\omega_0}, \frac{\omega_2}{\omega_0}, \frac{\omega_3}{\omega_0}, \frac{\omega_4}{\omega_0}, g\right)}{\tilde{\Gamma}\left(\frac{\omega_1}{\omega_0'}, \frac{\omega_2}{\omega_0'}, \frac{\omega_3}{\omega_0'}, \frac{\omega_4}{\omega_0'}, g'\right)} \cdot \frac{d^2\left(\frac{\omega}{\omega_0}, g\right)}{d^2\left(\frac{\omega}{\omega_0'}, g'\right)} \qquad /2.9/$$

is called invariant coupling. Neglecting the imaginary parts of the Green's function and vertices, the denominator of /2.9/ can be normalized to unity at $\omega = \omega_0'$ and the usual definition of the invariant coupling is recovered.

$$g_{inv} = g \, \tilde{\Gamma}\left(\frac{\omega_0'}{\omega_0}, g\right) d^2\left(\frac{\omega_0'}{\omega_0}, g\right). \qquad /2.10/$$

The denominator in eq. /2.9/ will be very important in what follows to show that g' is real and independent of the frequencies, as expected. Although $g_{inv} = g\tilde{\Gamma} d^2$

is the combination which is invariant under multiplicative renormalization, it is in general complex and the physically meaningful quantity is g'. With its knowledge several physical quantities can be calculated by solving a Lie differential equation.

Let A be a physical quantity which depends on the relative energy ω/ω_0 and obeys multiplicative renormalization, i.e.

$$A\left(\frac{\omega}{\omega_0'},\, g'\right) = z\left(\frac{\omega_0'}{\omega_0},\, g\right) A\left(\frac{\omega}{\omega_0},\, g\right). \qquad /2.11/$$

This equation can be cast into a differential form

$$\frac{\partial}{\partial x} \ln A(x, g) = \frac{1}{x} \frac{\partial}{\partial \xi}\left[\ln A(\xi, g'(x, g))\right]_{\xi = 1}, \qquad /2.12/$$

where $x = \omega/\omega_0$. According to this Lie equation the behaviour of A at x is governed by the behaviour of the invariant coupling g' at the same x. From a series expansion of the right-hand side of this equation in terms of the invariant coupling, the integration of eq. /2.12/ yields a summed up expression for A. This procedure keeping the first few terms of the series expansion gives a reasonable approximation in that case only if the invariant coupling is small in the interesting energy range, which, unfortunately, is not true for many problems and therefore only qualitative conclusions can be drawn from the results of this method.

It should be emphasized that the usual multiplicative renormalization procedure with introduction of the extra variable λ is more general than the treatment presented here. In the case of Anderson's model of dilute magnetic alloys, for example, where simple scale transformation can be done approximately only[16], the standard multiplicative renormalization technique has to be used[17].

III. X-ray absorption problem

As a simple example we will treat very briefly the x-ray absorption problem. The reader is referred to the papers[6,7] by Nozières et al. for the physical problem and for the notations. Furthermore, as above, the renormalization of the deep-electron Green's function, $d(\omega)$ and the reduced vertex $\tilde{\Gamma}$ are defined by

$$\mathcal{G} = \mathcal{G}_0 d , \qquad /3.1/$$

and

$$\Gamma = g \tilde{\Gamma} . \qquad /3.2/$$

The cut-off energy is denoted by ξ_0 in this section. The vertex will be calculated in a special case, namely when the energy of the conduction electrons is fixed at the Fermi energy and the remaining single variable is the deep-electron energy. It follows from the structure of the Dyson equation that the renormalization equations may have the form

$$G(\omega, \xi_0', g') = z_1 G(\omega, \xi_0, g), \qquad /3.3/$$

$$d\left(\frac{\omega}{\xi_0'}, g'\right) = z_2\, d\left(\frac{\omega}{\xi_0}, g\right), \qquad /3.4/$$

$$\tilde{\Gamma}\left(\frac{\omega}{\xi_0'}, g'\right) = z_3^{-1}\, \tilde{\Gamma}\left(\frac{\omega}{\xi_0}, g\right), \qquad /3.5/$$

$$g' = z_1^{-1} z_2^{-1} z_3\, g. \qquad /3.6/$$

First we have to show that these equations can be satisfied and then its consequences can be explored.

The graphs of the response function or those of the vertex must not contain deep-electron closed loops, i.e. no conduction-electron self-energy has to be included in these diagrams. In other words the conduction-electron Green's function G should remain unrenormalized in calculating these quantities and therefore $z_1=1$. For the deep-electron Green's function and the vertex we get

$$d(\omega) = 1 + g^2\left[\ln\frac{\omega}{\xi_0} - i\pi\,\Theta(\omega)\right] + \dots, \qquad /3.7/$$

$$\tilde{\Gamma}(\omega) = 1 - g^2\left[\ln\frac{\omega}{\xi_0} - i\pi\,\Theta(\omega)\right] + \dots, \qquad /3.8/$$

where $\Theta(\omega)$ is the step function. The self-consistent solution of eqs. /3.3/-/3.6/ using eqs. /3.7/ and /3.8/ is

$$z_2^{-1} = 1 + g^2 \ln\frac{\xi_0'}{\xi_0} + \dots, \qquad /3.9/$$

$$Z_3 = 1 - g^2 \ln \frac{\xi_0'}{\xi_0} + \dots , \qquad /3.10/$$

$$g' = g + \mathcal{O}(g^3) . \qquad /3.11/$$

The renormalizing factors and the new couplings are in fact real, though $d(\omega)$ and $\tilde{\Gamma}$ are complex. Applying the Lie equation for the invariant coupling itself, we get easily

$$g' = g , \qquad /3.12/$$

i.e. the coupling is not renormalized in the x-ray absorption problem. That is the probable reason why this problem can be solved exactly[18].

The response function

$$\chi(\omega) = -\left[\ln \frac{\omega}{\xi_0} - i\pi\Theta(\omega)\right] + g\left[\ln \frac{\omega}{\xi_0} - i\pi\Theta(\omega)\right]^2 + \dots \qquad /3.13/$$

does not satisfy the criterion of multiplicative renormalization, neither $\chi(\omega)/\chi^{(0)}(\omega)$, which is usually used in renormalization theory. This is probably due to the logarithmic nature of $\chi^{(0)}(\omega)$. Zawadowski[19] pointed out that the logarithmic derivative of χ is the proper quantity to be used for such a treatment. In fact

$$\bar{\chi}(\omega) = -\frac{1}{\omega}\frac{\partial \chi(\omega)}{\partial \omega} = 1 - 2g\left[\ln \frac{\omega}{\xi_0} - i\pi\Theta(\omega)\right] + \dots \qquad /3.14/$$

has good transformation properties. The Lie equation up to first order and its solution are

$$\frac{\partial \ln \bar{\chi}(x)}{\partial x} = -\frac{1}{x} 2g , \qquad /3.15/$$

$$\bar{\chi}(x) = C \exp(-2g \ln x) = C x^{-2g} , \qquad /3.16/$$

with $x = \omega/\xi_0$. By integrating $\bar{\chi}(x)$ and determining the constant of integration from fitting to the perturbational expression, we get

$$\chi(\omega) = \frac{1}{2g}\left[\left(\frac{\xi_0}{\omega}\right)^{2g} - 1\right] + i\pi\,\Theta(\omega)\left(\frac{\xi_0}{\omega}\right)^{2g} . \qquad /3.17/$$

This is precisely the result of the self-consistent treatment of the x-ray absorption problem in the weak coupling limit. The remarkable feature of the calculation is its simplicity. The power law singularity comes out in a natural way.

Analogously we get for the deep-electron Green's function

$$d(\omega) = \left[1 - i\pi g^2\,\Theta(\omega)\right]\left(\frac{\omega}{\xi_0}\right)^{g^2} , \qquad /3.18/$$

which again corresponds to the result of the self--consistent treatment.

Zawadowski[5] used another method to determine the imaginary part of the Green's function. He performed the renormalization for $\omega<0$ where the imaginary parts vanish and made an analytic continuation to $\omega>0$.

$$d(\omega<0) = \exp\left\{ g^2 \ln \frac{-\omega}{\xi_0} \right\} , \qquad /3.19/$$

and therefore

$$d(\omega>0) = \exp\left\{ g^2\left(\ln \frac{\omega}{\xi_0} - i\pi\right)\right\} = e^{-i\pi g^2}\left(\frac{\omega}{\xi_0}\right)^{g^2} . \qquad /3.20/$$

The Green's function obtained by this procedure has correct analytic properties. In the weak coupling limit the same form is reproduced as above.

IV. Scaling in the Kondo problem

In Abrikosov's[20] pseudofermion representation for the spin operators the Hamiltonian of the Kondo model is

$$H_{int} = \frac{J}{2N} \sum_{\substack{k,k' \\ \alpha\beta\gamma\delta}} b_\alpha^+ S_{\alpha\beta} b_\beta a_{k\gamma}^+ \sigma_{\gamma\delta} a_{k'\delta} + \frac{V}{2N} \sum_{\substack{k,k' \\ \alpha\beta}} b_\alpha^+ b_\alpha a_{k\beta}^+ a_{k'\beta} \qquad /4.1/$$

The potential scattering term has been included as in a consistent renormalization procedure V has to be taken into account throughout the calculation even if it is put equal to zero at the end.

We can proceed similarly as for the x-ray absorption problem and perform a multiplicative renormalization of the reduced vertices $\tilde{\Gamma}$,

$$\Gamma_{\alpha\beta\gamma\delta} = \frac{J}{2} \tilde{\Gamma}_\sigma (S_{\alpha\beta} \sigma_{\gamma\delta}) + \frac{V}{2} \tilde{\Gamma}_0 \delta_{\alpha\beta} \delta_{\gamma\delta} , \qquad /4.2/$$

of the conduction-electron Green's function G and of the pseudofermion Green's function $\mathcal{G} = \mathcal{G}_0 d$ by real factors z_i.

We assume that multiplicative renormalization can be achieved in this case as well, by a change of the cut-off energy D, i.e.

$$G(\omega, D', J', V') = z_1 G(\omega, D, J, V) , \qquad /4.3/$$

$$d(\omega, D', J', V') = z_2\, d(\omega, D, J, V), \qquad /4.4/$$

$$\tilde{\Gamma}_\sigma(\omega, D', J', V') = z_3^{-1}\, \tilde{\Gamma}_\sigma(\omega, D, J, V), \qquad /4.5/$$

$$\tilde{\Gamma}_0(\omega, D', J', V') = z_4^{-1}\, \tilde{\Gamma}_0(\omega, D, J, V), \qquad /4.6/$$

$$J' = z_1^{-1} z_2^{-1} z_3\, J, \qquad /4.7/$$

$$V' = z_1^{-1} z_2^{-1} z_4\, V. \qquad /4.8/$$

It is not at all trivial that these relations can be satisfied with real multiplicative factors, independent of the frequency variables. We will show that, at least up to a certain order, this scaling and multiplicative renormalization are consistent.

Similarly as in the x-ray problem, there is no self-energy correction on the conduction-electron lines inside any diagram and therefore $z_1=1$. The invariant couplings are defined as before, as the self-consistent solutions of the equations

$$J'\left(\frac{D'}{D}, J, V\right) = J\, \frac{\tilde{\Gamma}_\sigma(\omega, D, J, V)}{\tilde{\Gamma}_\sigma(\omega, D', J', V')}\, \frac{d(\omega, D, J, V)}{d(\omega, D', J', V')}, \qquad /4.9/$$

$$V'\left(\frac{D'}{D}, J, V\right) = V\, \frac{\tilde{\Gamma}_0(\omega, D, J, V)}{\tilde{\Gamma}_0(\omega, D', J', V')} \cdot \frac{d(\omega, D, J, V)}{d(\omega, D', J', V')}. \qquad /4.10/$$

Again the denominators in eqs. /4.9/ and /4.10/ cancel the imaginary parts and the frequency dependences of the corresponding numerators. This is demonstrated first for the parquet diagrams. The vertex contribution is calculated up to third order in two limiting cases,

namely when a/ the conduction-electron energy ε or b/ the pseudofermion energy ω is retained as single variable. In case a/ we have

$$\begin{aligned}\tilde{\Gamma}_{\sigma}(\varepsilon) = 1 &- J\varrho\left(\ln\frac{\varepsilon}{D} - \frac{1}{2}i\pi\right) - i\pi V\varrho \,\mathrm{sign}\,\varepsilon \\ &+ J^2\varrho^2\left(\ln\frac{\varepsilon}{D} - \frac{1}{2}i\pi\right)^2 \\ &+ i\pi JV\varrho^2\left(\ln\frac{\varepsilon}{D} - \frac{1}{2}i\pi\right)\mathrm{sign}\,\varepsilon \\ &- \frac{1}{4}\pi^2 J^2\varrho^2 S(S+1) + \frac{1}{4}\pi^2 JV\varrho^2 \,\mathrm{sign}\,\varepsilon \\ &- \frac{3}{4}\pi^2 V^2\varrho^2 + \dots ,\end{aligned} \tag{4.11}$$

$$\begin{aligned}\tilde{\Gamma}_{0}(\varepsilon) = 1 &- \frac{1}{2}i\pi\frac{J^2}{V}\varrho\, S(S+1)\,\mathrm{sign}\,\varepsilon - \frac{1}{2}i\pi V\varrho\,\mathrm{sign}\,\varepsilon \\ &+ i\pi\frac{J^3}{V}\varrho^2 S(S+1)\ln\frac{\varepsilon}{D}\,\mathrm{sign}\,\varepsilon \\ &+ \frac{1}{4}\pi^2\frac{J^3}{V}\varrho^2 S(S+1)\,\mathrm{sign}\,\varepsilon - \frac{3}{4}\pi^2 J^2\varrho^2 S(S+1) \\ &- \frac{1}{4}\pi^2 V^2\varrho^2 + \dots ,\end{aligned} \tag{4.12}$$

while in case b/

$$\begin{aligned}\tilde{\Gamma}_{\sigma}(\omega) = 1 &- J\varrho\left[\ln\frac{\omega}{D} - i\pi\,\Theta(\omega)\right] \\ &+ J^2\varrho^2\left[\ln\frac{\omega}{D} - i\pi\,\Theta(\omega)\right]^2 + \dots ,\end{aligned} \tag{4.13}$$

$$\tilde{\Gamma}_{0}(\omega) = 1 + \mathcal{O}(J^3, V^3) \tag{4.14}$$

is obtained. In the parquet approximation the pseudofermion lines are not renormalized, $d(\omega)=1$ and therefore $z_2=1$.

Taking any of these particular choices of the variables, the same expressions are obtained for the multiplicative factors z_i and for the invariant couplings:

$$z_3 = 1 - J\rho \ln \frac{D'}{D} + J^2 \rho^2 \ln^2 \frac{D'}{D} + \dots , \qquad /4.15/$$

$$J' = J \left(1 - J\rho \ln \frac{D'}{D} + J^2 \rho^2 \ln^2 \frac{D'}{D} + \dots \right) , \qquad /4.16/$$

$$V' = V . \qquad /4.17/$$

This fact confirms a posteriori our original assumption that multiplicative renormalization can be achieved by scaling the cut-off energy and that the invariant couplings are independent of the frequency variables. Inserting eq. /4.16/ into the Lie equation /2.12/, simple integration gives

$$J'\left(\frac{D'}{D}\right) = \frac{J}{1 + J\rho \ln \frac{D'}{D}} . \qquad /4.18/$$

This result could have been obtained from first-order scaling already, i.e. taking the first corrections to the invariant couplings and solving the Lie equation in that approximation. This shows that, as far as the invariant couplings are concerned, first-order scaling is equivalent to the parquet approximation. Unfortunately this is not the case for the observable physical quantities.

It is noteworthy that by considering the imaginary parts as well, the invariant couplings remain intact, while the scattering matrices change drastically. The spinflip and spin non-flip parts of the scattering matrix, τ and t, respectively, are known in the parquet approximation from the works of Hamann[21] and of Brenig and Götze[22]

$$\tau(\omega) = \frac{1}{\sqrt{\ln^2 \frac{\omega}{iT_K} + \pi^2 S(S+1)}} , \qquad /4.19/$$

$$t(\omega) = \frac{1}{2\pi i}\left[\frac{\ln \frac{\omega}{iT_K}}{\sqrt{\ln^2 \frac{\omega}{iT_K} + \pi^2 S(S+1)}} - 1\right] \qquad /4.20/$$

where the Kondo temperature is given by

$$1 + J\varrho \ln \frac{T_K}{D} = 0. \qquad /4.21/$$

The scattering amplitudes can be expressed in terms of the invariant coupling and we get

$$\tau(x) = \frac{1}{\sqrt{\left(1/J'(x) - \frac{1}{2} i\pi\right)^2 + \pi^2 S(S+1)}} , \qquad /4.22/$$

$$t(x) = \frac{1}{2\pi i}\left[\frac{1/J'(x) - \frac{1}{2} i\pi}{\sqrt{\left(1/J'(x) - \frac{1}{2} i\pi\right)^2 + \pi^2 S(S+1)}} - 1\right], \qquad /4.23/$$

where $x = \frac{\omega}{D}$. The logarithmic derivatives of these expressions are rather involved functions which, when expanded, include arbitrarily high powers of $J'/x/$. Due to these terms, first or second-order scaling is not sufficient for τ or t. As the invariant coupling, $J'/x/$ is divergent at the Kondo energy in this approximation, an infinite series summation is necessary to get non-singular behaviour for the observable quantities at T_K.

Lower-order logarithmic terms come not only from the imaginary parts but from the real contributions of non-parquet diagrams as well. Going beyond the parquet approximation, new corrections will appear in the invariant coupling, too. In calculating the third-order non-parquet vertex corrections, we have retained the energy of the pseudofermions, ω, as single variable.

$$\tilde{\Gamma}_\sigma(\omega) = 1 - J\varrho\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right] + J^2\varrho^2\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right]^2 - \frac{1}{2}\left\{J^2\varrho^2\left[S(S+1)-1\right] + V^2\varrho^2\right\}\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right] + \dots \qquad /4.24/$$

$$\tilde{\Gamma}_o(\omega) = 1 - \frac{1}{2}\left\{J^2\varrho^2 S(S+1) + V^2\varrho^2\right\}\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right] + \dots \qquad /4.25/$$

In this approximation the pseudofermion line is also renormalized,

$$d(\omega) = 1 + \frac{1}{2}\left\{J^2\varrho^2 S(S+1) + V^2\varrho^2\right\}\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right] + \dots \qquad /4.26/$$

The self-consistent solution of eqs. /4.4/-/4.8/, making use of eqs. /4.24/-/4.26/, is

$$z_2^{-1} = 1 + \frac{1}{2}\left\{J^2\varrho^2 S(S+1) + V^2\varrho^2\right\}\ln\frac{D'}{D} + \dots , \qquad /4.27/$$

$$z_3 = 1 - J\varrho\ln\frac{D'}{D} + J^2\varrho^2\ln^2\frac{D'}{D} - \frac{1}{2}\left\{J^2\varrho^2\left[S(S+1)-1\right] + V^2\varrho^2\right\}\ln\frac{D'}{D} + \dots , \qquad /4.28/$$

$$z_4 = 1 - \frac{1}{2}\left\{J^2\varrho^2 S(S+1) + V^2\varrho^2\right\}\ln\frac{D'}{D} + \dots , \qquad /4.29/$$

$$J' = J\left[1 - J\varrho \ln\frac{D'}{D} + J^2\varrho^2 \ln^2\frac{D'}{D} + \frac{1}{2} J^2\varrho^2 \ln\frac{D'}{D} + \dots\right], \qquad /4.30/$$

$$V' = V. \qquad /4.31/$$

The non-parquet diagrams give important contribution to the Lie equation for the invariant coupling,

$$\frac{\partial}{\partial x} \ln J'(x) = \frac{1}{x}\left[- J'(x)\varrho + \frac{1}{2} J'^2(x)\varrho^2 + \dots\right], \qquad /4.32/$$

$$\frac{\partial}{\partial x} \ln V'(x) = 0. \qquad /4.33/$$

This is the same Lie equation as obtained by Abrikosov and Migdal[3] and by Fowler and Zawadowski[4]. Abrikosov and Migdal[3] have calculated explicitely also the term proportional to J'^3 in eq. /4.32/.

From the present treatment which is more rigorous than theirs the following conclusions can be drawn: scaling of the cut-off energy is equivalent in the Kondo problem to multiplicative renormalization with real multiplicative factors; the invariant couplings are real, the imaginary parts of the Green's functions and vertices have no bearing on them and consequently, as before, the exchange coupling and the potential scattering are not coupled to each other, the potential scattering is not renormalized.

So far the isotropic Kondo problem has been investigated. Anderson's original scaling laws were derived for the anisotropic Kondo model. Zawadowski and the present author[10] extended Anderson's "poor man's method" to higher orders. The scaling laws obtained in that way agree with eq. /4.32/ in the isotropic case. Several points of that calculation, however, have not been clarified completely. One of them is the choice of the renormalized matrix element of the T matrix. The other problems were connected with the imaginary parts, which have been neglected everywhere, and with the choice of the energy variables in the scattering matrix. We will show in the Appendix that a consequent application of the renormalization group method yields automatically real invariant couplings for the anisotropic Kondo problem, too, and the same scaling laws are obtained as in Ref. 10.

V. Discussion

In the present paper a simple formulation of the multiplicative renormalization procedure has been presented for logarithmic problems. It is suggested that for the Kondo problem, the x-ray absorption problem and for one-dimensional metallic systems multiplicative renormalization of the Green's functions, vertices and coupling constants is equivalent to the scaling of the cut-off energy. In these cases there is no need to introduce the dummy variable λ and an unambiguous definition of the invariant coupling can be given.

The results of the present paper can be summarized as follows. First, we have shown that scaling of the cut-off energy and multiplicative renormalization with real factors are in fact equivalent for the Kondo problem and x-ray absorption problem. The one-dimensional metallic systems have been investigated separately[14,15], where the absence of phase transition has been demonstrated. It has been shown that starting from complex Green's functions and vertices a real invariant coupling can be introduced which is independent of the frequency variables and depends on the scaling energy only. The described procedure is applicable to logarithmic problems only. It seems that the introduction of the dummy variable λ cannot be avoided in other cases.

Second, we have rederived the scaling laws both for the isotropic and anisotropic Kondo models by taking into account the imaginary parts of the Green's functions and vertices. It turns out that these imaginary parts do not modify the scaling laws and therefore the relations obtained by Abrikosov and Migdal[3] as well as by Fowler and Zawadowski[4] for the isotropic case and by Sólyom and Zawadowski[10] for the anisotropic one emerge intact. By this we have put the scaling theory of the Kondo problem on a more rigorous basis.

Provided the invariant coupling is known, it can be used in the Lie equation to determine observable physical quantities like susceptibility, resistivity etc. We have shown on the example of the scattering matrix that, although, in principle, the knowledge of the invariant coupling helps to determine the matrices τ and t, in reality all the skeleton graphs have to be calculated to get reasonable results. In these quantities the imaginary part of the parquet diagrams and the contribution of the nonparquet diagrams are of the same order of magnitude and they all have to be taken into account. No reliable theory exists as yet how to treat this problem. In lack of such a treatment only qualitative conclusions can be drawn from the renormalization group approach. For a detailed discussion of the scaling laws and their consequences the reader is referred to the papers of Abrikosov and Migdal[3], Fowler and Zawadowski[4], Anderson et al.[8] and Zawadowski and the present author[10].

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Appendix

The anisotropic Kondo Hamiltonian is written in the form

$$H_{int} = \frac{J_z}{2N} \sum_{\substack{k,k' \\ \alpha\beta\gamma\delta}} b_\alpha^+ S^z_{\alpha\beta} b_\beta a^+_{k\gamma} \sigma^z_{\gamma\delta} a_{k'\delta}$$

$$+ \frac{J_\pm}{2N} \sum_{\substack{k,k' \\ \alpha\beta\gamma\delta}} b_\alpha^+ b_\beta a^+_{k\gamma} a_{k'\delta} \left(S^+_{\alpha\beta} \sigma^-_{\gamma\delta} + S^-_{\alpha\beta} \sigma^+_{\gamma\delta} \right) \qquad /A.1/$$

$$+ \frac{V}{2N} \sum_{kk'\alpha\beta} b_\alpha^+ b_\alpha a^+_{k\beta} a_{k'\beta} .$$

In the particular case S=1/2 the structure of the full vertex is

$$\Gamma_{\alpha\beta\gamma\delta} = \frac{J_z}{2} \tilde{\Gamma}_z \left(S^z_{\alpha\beta} \sigma^z_{\gamma\delta} \right)$$

$$+ \frac{J_\pm}{2} \tilde{\Gamma}_\pm \left(S^+_{\alpha\beta} \sigma^-_{\gamma\delta} + S^-_{\alpha\beta} \sigma^+_{\gamma\delta} \right) + \frac{V}{2} \tilde{\Gamma}_0 \delta_{\alpha\beta} \delta_{\gamma\delta} . \qquad /A.2/$$

For general values of the spin the spin products in the higher-order terms can not be cast into the simple form of eq. /A.2/ and more invariant couplings ought to be introduced.

The following form is supposed for the scaling equations

$$G(\omega, D', J'_\pm, J'_z, V') = z_1 \, G(\omega, D, J_\pm, J_z, V) , \qquad /A.3/$$

$$d(\omega, D', J'_\pm, J'_z, V') = z_2 \, d(\omega, D, J_\pm, J_z, V) , \qquad /A.4/$$

$$\tilde{\Gamma}_\pm(\omega, D', J'_\pm, J'_z, V') = z_3^{-1} \tilde{\Gamma}_\pm(\omega, D, J_\pm, J_z, V) , \qquad /A.5/$$

$$\tilde{\Gamma}_z(\omega, D', J'_\pm, J'_z, V') = z_4^{-1} \tilde{\Gamma}_z(\omega, D, J_\pm, J_z, V) , \qquad /A.6/$$

$$\tilde{\Gamma}_0(\omega, D', J'_\pm, J'_z, V') = z_5^{-1} \tilde{\Gamma}_0(\omega, D, J_\pm, J_z, V) , \qquad /A.7/$$

$$J'_\pm = z_1^{-1} z_2^{-1} z_3 J_\pm , \qquad /A.8/$$

$$J_z' = z_1^{-1} z_2^{-1} z_4 J_z \,, \qquad /A.9/$$

$$V' = z_1^{-1} z_2^{-1} z_5 V \,, \qquad /A.10/$$

where, as before, the conduction-electron Green's function should not be renormalized and therefore $z_1=1$. The perturbational result for the pseudofermion Green's function and vertices is

$$d(\omega) = 1 + \frac{1}{4}\left[J_\pm^2 + \frac{1}{2}J_z^2 + 2V^2\right]\varrho^2\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right] + \dots \,, \qquad /A.11/$$

$$\tilde{\Gamma}_\pm(\omega) = 1 - J_z\varrho\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right] + \frac{1}{2}\left(J_\pm^2 + J_z^2\right)\varrho^2\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right]^2$$
$$+ \frac{1}{4}\left[\frac{1}{2}J_z^2 - 2V^2\right]\varrho^2\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right] + \dots \,, \qquad /A.12/$$

$$\tilde{\Gamma}_z(\omega) = 1 - \frac{J_\pm^2}{J_z}\varrho\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right] + J_\pm^2\varrho^2\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right]^2 \qquad /A.13/$$
$$+ \frac{1}{4}\left[J_\pm^2 - \frac{1}{2}J_z^2 - 2V^2\right]\varrho^2\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right] + \dots \,,$$

$$\tilde{\Gamma}_0(\omega) = 1 - \frac{1}{4}\left[J_\pm^2 + \frac{1}{2}J_z^2 + 2V^2\right]\varrho^2\left[\ln\frac{\omega}{D} - i\pi\Theta(\omega)\right] + \dots \qquad /A.14/$$

The self-consistent solution of these equations easily gives

$$J_\pm' = J_\pm\left\{1 - J_z\varrho\ln\frac{D'}{D} + \frac{1}{2}\left(J_\pm^2 + J_z^2\right)\varrho^2\ln^2\frac{D'}{D}\right.$$
$$\left. + \frac{1}{4}\left(J_\pm^2 + J_z^2\right)\varrho^2\ln\frac{D'}{D} + \dots\right\} \,, \qquad /A.15/$$

$$J_z' = J_z\left\{1 - \frac{J_\pm^2}{J_z}\varrho\ln\frac{D'}{D} + J_\pm^2\varrho^2\ln^2\frac{D'}{D} + \frac{1}{2}J_\pm^2\varrho^2\ln\frac{D'}{D} + \dots\right\} \,, \qquad /A.16/$$

$$V' = V \,. \qquad /A.17/$$

These expressions yield the same scaling laws as in Ref. 10,

$$\frac{\partial J'_{\pm}(x)}{\partial x} = \frac{1}{x}\left\{ - J'_{\pm} J'_{z} \rho + \frac{1}{4}\left(J'_{\pm} J'^{2}_{z} + J'^{3}_{\pm} \right) \rho^{2} + \dots \right\}, \qquad /A.18/$$

$$\frac{\partial J'_{z}(x)}{\partial x} = \frac{1}{x}\left\{ - J'^{2}_{\pm} \rho + \frac{1}{2} J'^{2}_{\pm} J'_{z} \rho^{2} + \dots \right\}, \qquad /A.19/$$

$$\frac{\partial V'(x)}{\partial x} = 0 \qquad /A.20/$$

These scaling laws have been discussed by Zawadowski and the present author[10]. Here we want to emphasize that fact that the imaginary parts of the Green's functions and vertices cancel out in the invariant couplings, they are real and independent of ω.

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