migration of either the crowdion or normal interstitial takes place below stage III, although both are created by low-energy electron irradiation in copper and aluminum. In the stage-I region the recovery is due to the correlated recombination of (100) displacements (normal interstitial) and defocused (110) long-range (LR) sequences (crowdions). The dose effects found in copper and aluminum at the end of stage I are due to the recombination of secondary pairs, where the interstitial created by an LR sequence recombines with the vacancy of another Frenkel pair, (or in a prequench case with the quenched-in vacancies). Experimentally the dose and prequench effects take place in a relatively narrow temperature range. This is explained by von Jan by assuming that the crowdion produced by a LR sequence converts into a normal interstitial, with an activation energy near 0.1 eV in copper for example, *before* it can migrate. After conversion the normal interstitial, of course, recombines with a vacancy if the recombination energy is less than the conversion energy. Uncorrelated or free migration of the normal interstitial takes place in stage III. The data presented here are qualitatively consistent with the model proposed by von Jan.

von Jan explains the relatively small stage-I recovery in gold as being due to the absence of (110) displacements. Consequently in light of the above discussion one would expect the displacement processes in platinum and gold to be different. From the results of the previous paper we see that this does not seem to be the case for 45 eV $<T_m<70$ eV. On the other hand the comparison of the gold and platinum damage rates in the preceding paper may not extend to sufficiently large values of T_m to permit a conclusive comparison on this matter. Clearly higher energy irradiation of gold is desirable.

In conclusion, the data presented here do not lead to an unambiguous choice between the various recovery models discussed in this paper.

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Derivation of Kondo Anomalous Scattering from the Anderson Dilute-Alloy Model

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The Anderson extra-orbital dilute-alloy model is shown to lead to the same type of anomalous conduction-electron scattering found by Kondo from the *s-d* exchange model. This is accomplished by evaluating the *d*-state Green's function to fourth order in the *s-d* mixing potential and in the limit of large repulsion between two *d*-state electrons, using equation-of-motion techniques.

1. INTRODUCTION

In a recent paper[1] (hereafter denoted I), the author showed that Anderson's dilute-alloy model[2] yields a Curie-law magnetic susceptibility when the mutual repulsion U between two electrons in the extra "d" orbital is large, and the d-state width is small compared with its binding energy. This result demonstrates that a virtual bound state can display at least one of the properties associated with a truly bound spin. It is known, however, that a truly bound spin in a metal displays another important property—the anomalous scattering of the conduction electrons found by Kondo.[3] In this paper, we extend the calculation of I to the next order, and demonstrate the existence of the Kondo anomalous scattering term for the Anderson model. Furthermore, the coefficient of this term is just that given by substituting the exchange constant found by Schrieffer and Wolff[4] through a canonical transformation of Anderson's Hamiltonian into Kondo's result.[3]

We do not attempt in this paper to reproduce the results of the more sophisticated treatments of Kondo's model,[5–9] but merely those of the perturbation-

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theoretic calculation.[3] Thus our result is valid only for temperatures well above the critical temperature $T_c \approx \epsilon_F \exp(-1/|J|\rho)$, where ϵ_F is the Fermi energy, J the exchange constant, and ρ the Fermi-surface density of states.[5] We feel, however, that this is the necessary next step towards understanding the behavior of the Anderson model. Only by studying the basic Kondo effect above T_c can the key contributions be singled out to find the path to follow towards obtaining a valid solution below T_c. In this sense, our calculation parallels the first half of Nagaoka's[5] (both using double-time Green's functions),[10] and it is possible to draw a number of correspondences between the two.

A type of anomalous scattering for the Anderson model significantly different from the Kondo effect has recently been reported by Kim.[11] This result arises from the fact that after decoupling his equation of motion (2.13), Kim retains the expectation value $\langle a_{k-}^\dagger a_{k-}\rangle$ and neglects $\langle a_{d-}^\dagger a_{k-}\rangle$. (The $a_{k\sigma}$ and $a_{d\sigma}$ are the annihilation operators for the band and d states, respectively.) It may be seen from I, Eqs. (5) and (6), that these expectation values contribute *equal and opposite* logarithmic singularities to the d-state Green's function to second order in V, the d-state mixing potential. Kim shows that this neglect can be justified when V is considered to be of the same order as the d-state binding energy. However, when V is not a small parameter, it is not clear that his low-order decoupling or his neglect of the sum over k' of $\langle a_{k'-}^\dagger a_{k-}\rangle$ compared with the diagonal term are reasonable approximations. Therefore we must remain skeptical about these results.

Other calculations of the d-state Green's function by Kjöllerström *et al.*[12] and by Hewson[13] have been concerned with the magnetic properties of the d state, and have not attempted to go to high enough order in V, the s-d mixing potential, to find the Kondo effect. A calculation by Dworin, the published results of which give logarithmic temperature dependencies for the susceptibility and specific heat,[14] should in principle give the correct anomalous scattering.

The philosophy of the present calculation is similar to that of I. We consider the large-U limit, dropping all contributions of order U^{-1} at an early stage. This is a physically interesting limiting case which is, in a sense, halfway between the Kondo and Anderson models. The d state can be singly occupied or empty, so that it is a virtual state with a spread in energy, but it cannot be doubly occupied. Since the impurities which actually display magnetic moments are transition or rare-earth elements, the nondegenerate Anderson model can only give a qualitative picture of the physics of real systems, and we feel that the large-U limit does equally well in this respect. A final reason for exploring this limit is that it reduces the number of equations of motion which must be studied to obtain the Kondo effect by an order of magnitude and brings the prospect of qualitatively understanding the results within the realm of possibility.

A feature of I which the present calculation does not contain is the self-consistent solution for the d-state occupation numbers in the presence of a magnetic field. This omission simplifies the computation considerably, but prevents an evaluation of the susceptibility. It is, however, in keeping with a program of attempting to find a solution of the Anderson model valid below T_c by analogy with solutions of the Kondo problem.

In Sec. 2, the method of obtaining the d-state Green's function is explained in detail and the result is given. A relation between the band state and d-state Green's functions is proved in Sec. 3, and some correlation functions occurring in the result of Sec. 2 are calculated. The leading terms which give the Kondo effect are evaluated in Sec. 4.

2. THE d-STATE GREEN'S FUNCTION

The Hamiltonian for the Anderson model is

$$H=\sum_\sigma \epsilon_d a_{d\sigma}^\dagger a_{d\sigma}+\sum_{k\sigma} \epsilon_k a_{k\sigma}^\dagger a_{k\sigma}+U n_{d+} n_{d-} + \sum_{k\sigma}(V_{kd} a_{k\sigma}^\dagger a_{d\sigma}+V_{kd}^* a_{d\sigma}^\dagger a_{k\sigma}). \quad (2.1)$$

The standard form for a Green's-function equation of motion, after Fourier transformation to the energy representation, is

$$\omega\langle\langle A\,|\,B\rangle\rangle=(1/2\pi)\langle\{A,B\}\rangle+\langle\langle[A,H]\,|\,B\rangle\rangle, \quad (2.2)$$

where we have used the notation of Ref. 10, and assume A and B are Fermion-like operator combinations so that the anticommutator $\{\ \}$ is appropriate in the first term on the right. All Green's functions in (2.2) have the energy argument ω. In the second term, the commutator with the one-particle diagonal part of H will give energies times the original Green's function, which may be taken to the left. This problem has a special feature, however. The commutator of an operator combination like $n_{d-}a_{d+}$ with the U term of H gives $Un_{d-}n_{d-}a_{d+} = Un_{d-}a_{d+}$. Hence U times the original Green's function can occur on the right in (2.2), and this term can also be moved to the left. The standard result of (2.2) can be written

$$G=(\omega-\text{energies})^{-1}[(1/2\pi)(\text{thermal average}) + (\text{coefficients and perhaps sums})(\text{new } G\text{'s})], \quad (2.3)$$

where G means Green's function. The difficulty in treating the Anderson model systematically using equations of motion is that the "coefficients" in (2.3) can be either the small quantity V_{kd} or the large quantity U. Therefore, proceeding n steps down the equation-of-motion

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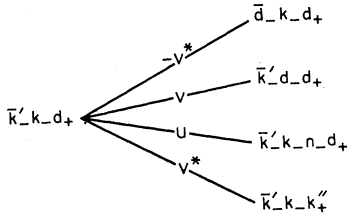

FIG. 1. Diagram summarizing a typical equation of motion.

hierarchy does not give all V^n contributions to the initial G, and the complexity of the set of equations which must be dealt with to get even the V^4 terms is appalling.

To cope with this, we have developed a graphical technique for representing the equations of motion which enables us to exploit the large-U approximation and reduce drastically the number of equations which need actually be written down. Before explaining this, it will be helpful to introduce the notation which will be used in the rest of this paper by a few examples. For Green's functions:

$$\begin{aligned} G(d_+) &\equiv \langle\langle a_{d+} | a_{d+}^\dagger \rangle\rangle, \\ G(d_+;\bar{k}_+) &\equiv \langle\langle a_{d+} | a_{k+}^\dagger \rangle\rangle, \\ G(\bar{d}_-k_-d_+) &\equiv \langle\langle a_{d-}^\dagger a_{k-} a_{d+} | a_{d+}^\dagger \rangle\rangle, \\ G(\bar{k}''_-k_-n_-d_+) &\equiv \langle\langle a_{k''-}^\dagger a_{k-} n_{d-} a_{d+} | a_{d+}^\dagger \rangle\rangle. \end{aligned} \tag{2.4}$$

It should be noted that the operator on the right is assumed to be $a_{d+}^\dagger$ unless the argument of G contains a semicolon. In addition, all Green's functions are understood to have the same energy argument ω. For thermal averages:

$$\begin{aligned} \langle \bar{d}_-k_- \rangle &\equiv \langle a_{d-}^\dagger a_{k-} \rangle, \\ \langle \bar{d}_-\bar{k}''_+k_-k_+' \rangle &\equiv \langle a_{d-}^\dagger a_{k''-}^\dagger a_{k-} a_{k'+} \rangle. \end{aligned} \tag{2.5}$$

For energy denominators:

$$\begin{aligned} D(d) &= (\omega - \epsilon_d)^{-1}, \\ D(\bar{d}kk') &= (\omega + \epsilon_d - \epsilon_k - \epsilon_{k'})^{-1}, \\ D(\bar{k}''dk') &= (\omega + \epsilon_{k''} - \epsilon_d + \epsilon_{k'})^{-1}. \end{aligned} \tag{2.6}$$

The existence of identities such as $D(\bar{d}kd) = D(k)$ and the permutability of the arguments of the D's should also be noted. The final bit of notation we shall introduce is that of parenthesized superscripts to indicate the order in V to which a Green's function or thermal average should be evaluated. Thus $G^{(0)}(d_+)$ and $\langle \bar{d}_-k_- \rangle^{(1)}$ should be evaluated in zeroth and first order, respectively.

To introduce the graphical notation, let us first look at a typical equation of motion which occurs in the hierarchy for $G(d_+)$,

$$\begin{aligned} G(\bar{k}'_-k_-d_+) = D(k'kd)[&(1/2\pi)\langle \bar{k}'_-k_- \rangle \\ &- V_{k'd}{}^* G(\bar{d}_-k_-d_+) + V_{kd} G(\bar{k}'_-d_-d_+) \\ &+ UG(\bar{k}'_-k_-n_-d_+) + \sum_{k''} V_{k''d}{}^* G(\bar{k}'_-k_-k''_+)]. \end{aligned} \tag{2.7}$$

Now we note that the "important" information in this equation is contained in the arguments of the G's on the right and their coefficients. The arguments of D and of the thermal average can be obtained immediately by inspection of the G on the left. Therefore, (2.7) can be conveniently summarized by a diagram such as that shown in Fig. 1. The rules for drawing such a diagram are extremely simple. One takes each argument of the initial G in turn and applies Fig. 2. One then scans the list of new arguments for combinations of d and n operators which are zero (i.e., $n_+d_+=0$) or which simplify (i.e., $d_+n_+=d_+$, $n_-n_-=n_-$), and either writes 0 next to or makes a correction by erasure to the appropriate terms. Care must be taken to add primes to new k arguments. A new set of branches can now be drawn from each nonzero new argument, etc., so that the original G forms the trunk from which a tree of branches grows. One economy which can be achieved immediately in this process is to write T (for terminates) next to any argument that has occurred to the left in the tree, drawing no further branches from that point.

Next we must consider the utility of the graphical technique in making approximations. The key approximation is based on considering U large compared to other energies in the problem. Figure 3 shows the two possible configurations involving U that can occur in the tree. In both, the argument list B is connected to itself by a U line, forming a terminating branch. The equation for $G(B)$ will contain $UG(B)$ on its right, so this term will be moved to the left and U will be taken into the energy denominator. Since U is large, we may replace the D in the $G(B)$ equation by $(-1/U)$. In Fig. 3(a), B is connected to A by a V line. Thus it makes a contribution of order U^{-1} to $G(A)$ and everything to its left and should be dropped. In Fig. 3(b) on the other hand, B is connected to C by a U line and makes a contribution of order unity in U to $G(C)$ and everything to

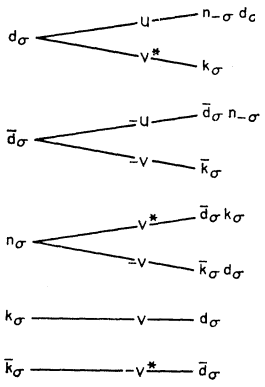

FIG. 2. Illustration of the rules for constructing diagrams to represent equations of motion.

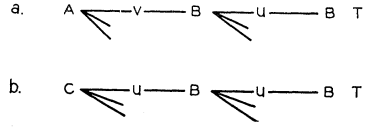

FIG. 3. Possible configurations in a diagram representing a chain of equations of motion. A, B, and C are argument lists.

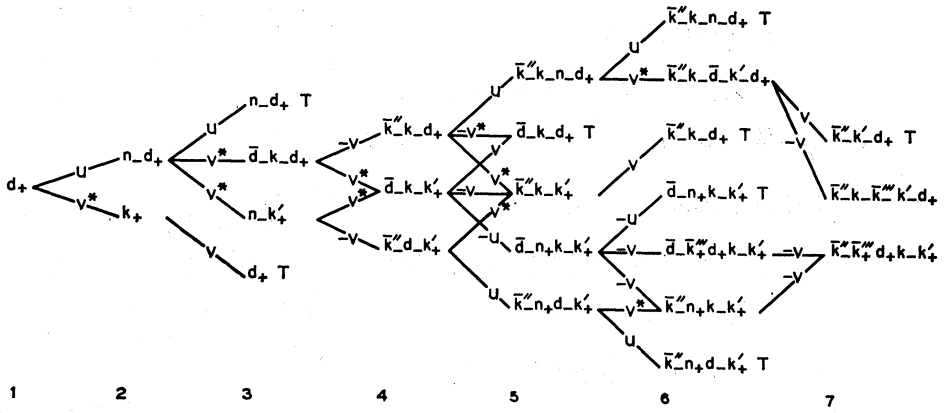

FIG. 4. Diagram summarizing the chain of equations of motion needed to obtain $G(d_+)$ correctly to order V^4.

its left. In this configuration, B must be kept. A third configuration, in which an argument list has a U line to its left and only V lines or a U line to a different list to its right, cannot occur. Making this approximation as the tree is being drawn simplifies it enormously.

In I, we noted the importance of keeping *all* terms which contribute to a given order of V in $G(d_+)$ because of the cancellation of terms which by themselves were singular. The diagram method makes this easy. To obtain all V^4 contributions to $G(d_+)$, we first draw its tree until all rightmost "leaves" are connected to the trunk by five V branches. (U branches which occur on the path from a leaf to the trunk are not counted.) Then we erase all these leaves and their branches. Next, we examine each remaining rightmost leaf and decide whether the thermal average term in its equation of motion contains any contribution of zero order in V. (For example $\langle \bar{k}'''\_k''\_\bar{k}'\_+k_+\rangle$ does, but $\langle \bar{k}'''\_k''\_\bar{d}\_+k_+\rangle$ does not.) If not, we erase it and its branch and continue to examine any new rightmost leaves. For those rightmost leaves tagged T, we first count the number N of V lines to the trunk. We then examine the tree growing from the first occurrence of this leaf, and decide whether it contains contributions of order $4-N$ or less. If not, we erase this "T-leaf" and continue. After the tree has been pruned in this manner, we examine argument lists on the same vertical line. If any are identical, it is then possible to condense the diagram, perhaps relabeling some k arguments. The redrawn diagram will then have several lines entering some of the argument lists from the left.

This program was carried out to order V^4, and the result is shown in Fig. 4. It should be noted that the word "decoupling," so common in most calculations using double-time Green's functions, was never used in the preceding discussion. We abandoned this usual method of terminating the hierarchy of equations after observing that it often led to erroneous results due to the presence of the large parameter U in the Anderson Hamiltonian. In some cases, decoupling does give the correct result. In particular, the zero-order contributions to each Green's function represented in column 7 of Fig. 4 are given correctly by decoupling. It is for this reason that we have omitted columns 8 and 9, which are present in the original diagram drawn according to prescription.

To evaluate $G^{(4)}(d_+)$, we write an equation of motion for every G represented in Fig. 4 which has a line going to its right, working from right to left and substituting as we go. As in I, we avoid placing self-energies in denominators for two reasons: First, the behavior of $G(d_+)$ near its unperturbed pole at $\omega=\epsilon_d$ is not important. For the Kondo effect, as in the Curie-law calculation, only the behavior of $G(d_+)$ near $\omega=0$ is important. Second, as in I, cancellations of discontinuous and singular functions are important, so we must keep our expansion in powers of V a strict one. For example, we might observe that the equation of motion for $G(\bar{d}\_k\_d_+)$ from column 3 will contain the same G on its right from column 5, and that we could combine this term with the energy denominator. In keeping with the strict expansion principle, however, we should treat the terms in question as $G^{(3)}(\bar{d}\_k\_d_+)$ in column 3 and $G^{(1)}(\bar{d}\_k\_d_+)$ in column 5, that is, as different functions. When this is done, we find that other terms containing $G^{(1)}(\bar{d}\_k\_d_+)$ enter column 5 from columns 6 and 7, leading to some important cancellations.

The methods of evaluating the thermal averages which occur in the set of equations of motion will be discussed in the next section. The result is

$$G^{(4)}(d_+)=G^{(0)}(d_+)+D(d)\sum_{j=1}^{9}A_j, \tag{2.8}$$

where

$$A_1=\frac{1}{2\pi}\sum_k D(k)V_{kd}{}^*\langle\bar{d}\_k\_\rangle^{(3)}, \tag{2.9}$$

$$A_2=\frac{1}{2\pi}\sum_{kk''} D(k)D(\bar{k}''kd)V_{kd}{}^*V_{k''d} \times[\langle\bar{k}''\_k\_d\_\bar{d}\_\rangle^{(2)}-\langle k''\_\bar{d}\_+d\_k\_+\rangle^{(2)}], \tag{2.10}$$

$$A_3=\frac{|1}{2\pi}\sum_{kk'}[D(k)+D(k')]D(\bar{d}kk') \times V_{kd}{}^*V_{k'd}{}^*\langle\bar{d}_-\bar{d}_+k_-k'_+\rangle^{(2)}, \quad (2.11)$$

$$A_4=G^{(0)}(d_+)\sum_k D(k)|V_{kd}|^2, \quad (2.12)$$

$$A_5=D(d)\sum_{kk'}(1+n_{k-})|V_{kd}|^2D(k)V_{k'd}{}^* \times[V_{k'd}D(k')G^{(0)}(d_+)-G^{(1)}(\bar{d}_-k'_-d_+)], \quad (2.13)$$

$$A_6=-\sum_{kk''}(1-n_{k''-})|V_{k''d}|^2[D(\bar{k}''kd) +D(\bar{d}kk'')]D(k)V_{kd}{}^*G^{(1)}(\bar{d}_-k_-d_+), \quad (2.14)$$

$$A_7=-\sum_{kk'}(1-n_{k+})|V_{kd}|^2D(\bar{d}kk') \times D(k)V_{k'd}{}^*G^{(1)}(\bar{d}_-k'_-d_+), \quad (2.15)$$

$$A_8=\sum_{kk''}n_{k''-}|V_{k''d}|^2[D(\bar{k}''dk) +D(\bar{d}kk'')]D(k)V_{kd}{}^*F(k_+), \quad (2.16)$$

$$A_9=\sum_{kk'}n_{k-}|V_{kd}|^2D(\bar{d}kk')D(k)V_{k'd}{}^*F(k'_+). \quad (2.17)$$

The following notation is used in the above:

$$n_{k\sigma}=\langle\bar{k}_\sigma k_\sigma\rangle^{(0)}, \quad (2.18)$$

$$G^{(0)}(d_+)=(1/2\pi)D(d)[1-\langle n_-\rangle], \quad (2.19)$$

$$G^{(1)}(\bar{d}_-k_-d_+)=D(k)[(1/2\pi)\langle\bar{d}_-k_-\rangle^{(1)} -n_{k-}V_{kd}G^{(0)}(d_+)], \quad (2.20)$$

$$F(k_+)=D(k)[(1/2\pi)\langle\bar{d}_+k_+\rangle^{(1)} +(1-n_{k+})V_{kd}G^{(0)}(d_+)]. \quad (2.21)$$

In the above equations, spin indices have been retained and the effects of a magnetic field $\mathfrak{IC}$ can be included simply by adding $\mu_B\mathfrak{IC}$ to each energy denominator D^{-1}, where μ_B is the Bohr magneton. The terms in $G^{(4)}(d_+)$ will be discussed in Sec. 4, and those giving the Kondo effect will be approximately evaluated.

3. BAND-STATE GREEN'S FUNCTION AND THERMAL AVERAGES

To relate the result for $G(d_+)$ to the Kondo effect and to evaluate some of the thermal averages which appear in it, we will prove an exact relation for the band-state Green's function $G(k_+;\bar{k}'_+)$. The equation of motion for this G is

$$G(k_+;\bar{k}'_+)=D(k)[(1/2\pi)\delta_{kk'}+V_{kd}G(d_+;\bar{k}'_+)]. \quad (3.1)$$

If we now form an equation of motion for the new G which appears in (3.1) by taking the time derivative with respect to the time argument of the *operator on the right*, we obtain

$$G(d_+;\bar{k}'_+)=D(k')V_{k'd}{}^*G(d_+). \quad (3.2)$$

Substituting (3.2) in (3.1),

$$G(k_+;\bar{k}'_+)=(1/2\pi)\delta_{kk'}D(k) +V_{kd}V_{k'd}{}^*D(k)D(k')G(d_+). \quad (3.3)$$

This is an exact result; any approximate evaluation of $G(d_+)$ will give the corresponding approximation for $G(k_+;\bar{k}'_+)$ directly using (3.3).

The quantity of interest in the Kondo effect is the self-energy of the diagonal Green's function $G(k_+;\bar{k}_+)$. By using (3.3) and the fact that $|V_{kd}|^2$ is inversely proportional to the system volume (which is unimportant everywhere else since $|V_{kd}|^2$ appears in k sums), we can show

$$[2\pi G(k_+;\bar{k}_+)]^{-1}=\omega-\epsilon_k-2\pi|V_{kd}|^2G(d_+), \quad (3.4)$$

which is valid for complex ω and may thence be continued to the real axis. For a finite concentration of impurities c, the self-energy is

$$\Sigma_k(\omega)=2\pi c|V_{kd}|^2G(d_+). \quad (3.5)$$

The theory of impurity averaging of Green's functions is a more satisfying way of reaching this reuslt.[15] The similarity in form between Eqs. (3.3) and (3.4) and Nagaoka's results using the Kondo Hamiltonian[5] should be noted. We see from (3.5) that the Kondo anomalous scattering,[3] which produces a logarithmic singularity in the imaginary part of $\Sigma_k(\omega)$ as ω approaches 0, should appear in a similar way in $\mathrm{Im}G(d_+)$.

In many of the equations of motion represented in Fig. 4, a thermal average occurs on the right. According to the general formalism of double-time Green's functions,[10] thermal averages are evaluated by using the prescription

$$\langle BA\rangle=i\int_{-\infty}^{\infty}[G(\omega+i\eta)-G(\omega-i\eta)]f(\omega)d\omega \equiv\mathfrak{F}[G], \quad (3.6)$$

where the G on the right is $G(A;B)$, η is a positive infinitesimal, and $f(\omega)$ is the Fermi function if A and B are Fermion-like operator combinations. Using

$$\mathfrak{F}[(1/2\pi)(\omega-\epsilon)^{-1}]=f(\epsilon), \quad (3.7)$$

the evaluation of thermal averages is extremely easy if the relevant G can be expanded in partial fractions in ω.

One difficulty attendant to the evaluation of more complicated thermal averages is the freedom possible in dividing the operators into A and B. Each choice calls for a different G, and it is not clear that approximate forms of these G's will all give the same result for the thermal average. Lacking a general answer to this difficulty, we proceeded according to the following principle: B was always chosen to be $\bar{d}_+$, so that G would be one of the Green's functions occurring in the set of equations of motion for $G^{(4)}(d_+)$. This choice is based on consistency and simplicity.

In the equations of motion from column 6 of Fig. 4, thermal averages such as $\langle \bar{k}''\_\bar{d}_+k\_k'_+\rangle^{(1)}$ occur. As can be easily verified, the obvious factorization is correct to this order, so

$$\langle \bar{k}''\_\bar{d}_+k\_k'_+\rangle = -\langle \bar{k}''\_k\_\rangle^{(0)}\langle \bar{d}_+k'_+\rangle^{(1)} = -\delta_{k''k}n_{k\_}\langle \bar{d}_+k'_+\rangle^{(1)}. \quad (3.8)$$

Such factorization was used in all first-order 4-operator averages, and is already present in the result of the last section.

The thermal average $\langle \bar{d}_+k'_+\rangle^{(1)}$ is easily evaluated from

$$G^{(1)}(k_+) = D(k)V_{kd}G^{(0)}(d_+). \quad (3.9)$$

Using (2.19), expanding in partial fractions, and applying (3.7), we find

$$\langle \bar{d}_+k_+\rangle^{(1)} = \mathfrak{F}[G^{(1)}(k_+)] = V_{kd}[1-\langle n_-\rangle]\frac{f(\epsilon_d)-f(\epsilon_k)}{\epsilon_d-\epsilon_k}. \quad (3.10)$$

In general, we may replace $f(\epsilon_d)$ by 1 in this and similar expressions.

It is clear that averages such as $\langle \bar{k}''\_\bar{d}_+d\_k_+\rangle^{(2)}$ which occur in column-5 equations of motion are not likely to be given correctly by factorization. Physically, this average represents the amplitude for a conduction electron and the local electron mutually flipping their spins, and Nagaoka found that such an average gives an important contribution to the anomalous scattering for the Kondo Hamiltonian.[5] We may evaluate this average from $G(\bar{k}''\_d\_k_+)$, which occurs in column 4 and is given by

$$G^{(2)}(\bar{k}''\_d\_k_+) = -D(\bar{k}''dk)[(1/2\pi)\langle \bar{k}''\_\bar{d}_+d\_k_+\rangle^{(2)} - n_{k''\_}V_{k''d}{}^*F(k_+)], \quad (3.11)$$

where F is defined in (2.21). Since the desired thermal average appears on the right in (3.11), using (3.6) yields an algebraic equation for it:

$$\langle \bar{d}_+\bar{k}''\_d\_k_+\rangle = f(\epsilon_d+\epsilon_k-\epsilon_{k''})\times\langle \bar{d}_+\bar{k}_-''d\_k_+\rangle + V_{k''d}{}^*V_{kd}[1-\langle n_-\rangle]\times[f(\epsilon_d)-f(\epsilon_d+\epsilon_k-\epsilon_{k''})]\frac{n_{k''}(1-n_k)}{(\epsilon_d-\epsilon_k)(\epsilon_{k''}-\epsilon_k)}. \quad (3.12)$$

Using $n_k=f(\epsilon_k)$ and substituting the explicit expression for the Fermi function enables us to show that

$$n_{k''}(1-n_k)\frac{f(\epsilon_d)-f(\epsilon_d+\epsilon_k-\epsilon_{k''})}{1-f(\epsilon_d+\epsilon_k-\epsilon_{k''})} = (n_{k''}-n_k)f(\epsilon_d), \quad (3.13)$$

so

$$\langle \bar{d}_+\bar{k}''\_d\_k_+\rangle^{(2)} = V_{k''d}{}^*V_{kd}\times[1-\langle n_-\rangle]\frac{n_{k''}-n_k}{(\epsilon_d-\epsilon_k)(\epsilon_{k''}-\epsilon_k)}, \quad (3.14)$$

where we set $f(\epsilon_d)=1$ on the right in (3.13). It clearly would have been unwise to make this approximation in (3.12). The singularity in (3.14) at $\epsilon_k=\epsilon_d$ is introduced by making the approximation $f(\epsilon_d)=1$ in evaluating $\langle \bar{d}_+k_+\rangle^{(1)}$ which is contained in F in (3.11). This step causes no difficulty in evaluating the leading terms in $G^{(4)}(d_+)$.

The average $\langle \bar{k}''\_k\_d\_\bar{d}\_\rangle^{(2)}$ which appears with (3.14) in (2.10) cannot be dealt with so easily. Examination of the arguments in Fig. 4 shows that it cannot be obtained from any of the G's which appear in the hierarchy. In order to evaluate this average let us write the identities

$$\langle \bar{k}''\_k\_d\_\bar{d}\_\rangle^{(2)} = \langle \bar{k}''\_k\_\rangle^{(2)} - \langle \bar{k}''\_k\_n\_\rangle^{(2)} \quad (3.15)$$

and

$$\langle \bar{k}''\_k\_n\_\rangle^{(2)} = \tfrac{1}{2}\langle \bar{k}''\_k\_(n_++n_-)\rangle^{(2)} - \tfrac{1}{2}\langle \bar{k}''\_k\_(n_+-n_-)\rangle^{(2)}. \quad (3.16)$$

To evaluate the second term in (3.16) we must use the invariance of the Anderson Hamiltonian, (2.1), under spin rotations. Doing so enables us to use the relations among thermal averages pointed out by Nagaoka for the Kondo model [his equation (2.13)],[5] in particular

$$-\tfrac{1}{2}\langle \bar{k}''\_k\_(n_+-n_-)\rangle = -\langle \bar{k}''\_k\_S_{dz}\rangle = \tfrac{1}{2}\langle \bar{k}''\_k{}_+S_{d+}\rangle = \tfrac{1}{2}\langle \bar{k}''\_k{}_+\bar{d}_+d\_\rangle, \quad (3.17)$$

where $\mathbf{S}_d$ is the d-state spin operator. The last line in (3.17) is just the average evaluated previously. We note that it is *only at this point* that we abandon the possibility of including a magnetic field and calculating the susceptibility as in I.

To obtain the first term on the right in (3.16), it would be physically reasonable to factor the average. However, we can do better. Let us consider

$$G^{(2)}(\bar{k}''\_k\_d_+) = \delta_{k''k}n_{k\_}D(d)\sum_{k'}V_{k'd}{}^*[V_{k'd}D(k')G^{(0)}(d_+) - G^{(1)}(\bar{d}\_k'\_d_+)] + D(\bar{k}''kd)[(1/2\pi)\langle \bar{k}''\_k\_d\_\bar{d}\_\rangle^{(2)} - (1-n_{k''\_})V_{k''d}{}^*G^{(1)}(\bar{d}\_k\_d_+)]. \quad (3.18)$$

It can be seen from I that the first term on the right in (3.18) is $\delta_{k''k}n_{k\_}[G^{(2)}(d_+)-G^{(0)}(d_+)]$. Applying the operator $\mathfrak{F}$ to (3.18), we find

$$\langle \bar{d}_+k''\_k\_d_+\rangle^{(2)} = f(\epsilon_d+\epsilon_k-\epsilon_{k''})\langle \bar{k}''\_k\_d\_\bar{d}\_\rangle^{(2)} + \delta_{k''k}n_k[\langle n\rangle^{(2)}-\langle n\rangle^{(0)}] + (1-\langle n\rangle)V_{k''d}{}^*V_{kd}\frac{(1-n_{k''})}{\epsilon_d-\epsilon_k}\left[\frac{n_k[f(\epsilon_d)-f(\epsilon_d+\epsilon_k-\epsilon_{k''})]}{\epsilon_{k''}-\epsilon_k} + \frac{f(\epsilon_k)-f(\epsilon_d+\epsilon_k-\epsilon_{k''})}{\epsilon_d-\epsilon_{k''}}\right], \quad (3.19)$$

where we have dropped the spin indices on n_k and $\langle n\rangle$ in keeping with setting the magnetic field equal to zero. By considering carefully the various Fermi functions in the last term on the right in (3.19), we see that it is small at the "suspicious" points $\epsilon_k\approx\epsilon_d$, $\epsilon_{k''}\approx\epsilon_d$, and $\epsilon_k\approx\epsilon_{k''}$ [compared to, say, (3.14) for small ϵ_k and $\epsilon_{k''}$]. Since one of the thermal averages we are investigating is large for these values of the argument, it is reasonable to take ϵ_k and $\epsilon_{k''}$ to be small in (3.19). Then $f(\epsilon_d+\epsilon_k-\epsilon_{k''})\approx 1$, and we obtain

$$\langle\bar{d}_+\bar{k}''_-k_-d_+\rangle^{(2)}+\langle\bar{k}''_-k_-\bar{d}_-d_-\rangle^{(2)}\equiv\langle\bar{k}''_-k_-(n_++n_-)\rangle^{(2)}$$
$$\approx\langle\bar{k}''_-k_-\rangle^{(2)}+\delta_{k''k}n_k[\langle n\rangle^{(2)}-\langle n\rangle^{(0)}]. \quad (3.20)$$

This is close to the result we would have obtained by decoupling. From (3.3), we find

$$\langle\bar{k}''_-k_-\rangle^{(2)}=\mathfrak{F}[G^{(2)}(k_-;\bar{k}''_-)]\approx\delta_{kk''}n_{k-}$$
$$-(1-\langle n\rangle)\frac{V_{kd}V_{k''d}^*}{\epsilon_d}\frac{n_{k''}-n_k}{\epsilon_{k''}-\epsilon_k}, \quad (3.21)$$

where the $\approx$ sign indicates we have kept only the large second-order term. Equation (3.21) substantiates our neglect of the last term on the right in (3.19), since it shows that the first term contains a much larger contribution.

Combining (3.17) and (3.21), we obtain for the combination of thermal averages needed in (2.10)

$$\langle\bar{k}''_-k_-d_-\bar{d}_-\rangle^{(2)}-\langle\bar{k}''_-\bar{d}_+d_-k_+\rangle^{(2)}=\tfrac{1}{2}\langle\bar{k}''_-k_-\rangle^{(2)}$$
$$-\tfrac{3}{2}\langle\bar{k}''_-k_+\bar{d}_+d_-\rangle+\tfrac{1}{2}\delta_{k''k}n_k[\langle n\rangle^{(2)}-\langle n\rangle^{(0)}]. \quad (3.22)$$

Substituting (3.21) and (3.14) (for small ϵ_k and $\epsilon_{k''}$) yields the explicit result

$$\langle k''_-k_-d_-\bar{d}_-\rangle^{(2)}-\langle\bar{k}''_-\bar{d}_+d_-k_+\rangle^{(2)}$$
$$=(1-\langle n\rangle)V_{kd}V_{k''d}^*\frac{1}{\epsilon_d}\frac{n_{k''}-n_k}{\epsilon_{k''}-\epsilon_k}$$
$$+\tfrac{1}{2}\delta_{k''k}n_k[1+\langle n\rangle^{(2)}-\langle n\rangle^{(0)}]. \quad (3.23)$$

The third 4-operator second-order thermal average entering $G^{(4)}(d_+)$ is $\langle\bar{d}_-\bar{d}_+k_-k'_+\rangle^{(2)}$, which appears in (2.11). We expect it to be small in our large-U limit. It can be calculated directly from $G^{(2)}(\bar{d}_-k_-k'_+)$ and is, in fact, small.

The remaining thermal average is $\langle\bar{d}_-k_-\rangle^{(3)}$, which can be computed in a straightforward manner:

$$\langle\bar{d}_\pm k_\pm\rangle^{(3)}=\mathfrak{F}[G^{(3)}(k_+)]$$
$$=\mathfrak{F}[V_{kd}D(k)G^{(2)}(d_+)]\approx\langle\bar{d}_\pm k_\pm\rangle^{(1)}$$
$$+2(1-\langle n\rangle)\frac{V_{kd}}{\epsilon_d^2}\sum_{k'}|V_{k'd}|^2\frac{n_{k'}-n_k}{\epsilon_{k'}-\epsilon_k}, \quad (3.24)$$

where the leading term has been extracted as before.

4. LEADING TERMS AND THE KONDO EFFECT

As pointed out in the discussion following (3.5), we expect the Kondo effect to manifest itself as a $\ln\omega$ singularity in the imaginary part of $G(d_+)$. Since Schrieffer and Wolff have shown that the Kondo model $J=2|V_{kF d}|^2/\epsilon_d$ at the Fermi surface in the Anderson model[4] and the $\ln\omega$ singularity appears with a J^3 coefficient in Kondo's calculation,[3] we expect from (3.5) a V^4 coefficient multiplying the $\ln\omega$ term in $\mathrm{Im}G(d_+)$. With this in mind, we shall examine the fourth-order contribution to each term in $G^{(4)}(d_+)$. (We showed in I that second-order terms give no anomalous contribution.)

The first term in the list of A's following (2.8) is evaluated using (3.24):

$$A_1=-\frac{1}{2\pi}2(1-\langle n\rangle)\frac{1}{\epsilon_d^2}$$
$$\times\sum_{kk'}|V_{kd}|^2|V_{k'd}|^2D(k)\frac{n_k-n_{k'}}{\epsilon_k-\epsilon_{k'}}. \quad (4.1)$$

The k' sum in (4.1) is not singular; it is well defined without adding an infinitesimal imaginary term to the denominator $(\epsilon_k-\epsilon_{k'})$ because of the presence of the numerator $(n_k-n_{k'})$, and is real. However, assuming a constant $V_{k'd}$ and a constant density of states ρ from $-\epsilon_F$ to ϵ_F, we find that at temperature $T=0$,

$$\sum_{k'}|V_{kd}|^2\frac{n_k-n_{k'}}{\epsilon_k-\epsilon_{k'}}=\rho V^2\ln\frac{|\epsilon_k|}{|\epsilon_k|+\epsilon_F}$$
$$\approx\rho V^2\ln|\epsilon_k/\epsilon_F|. \quad (4.2)$$

From (2.8), it is clear that for small ω

$$\mathrm{Im}G^{(4)}(d_+)=\mathrm{Im}D(d)\sum_{j=1}^{9}A_j\approx-\frac{1}{\epsilon_d}\sum_{j=1}^{9}\mathrm{Im}A_j. \quad (4.3)$$

We will consider the retarded Green's function, so that ω is replaced by $\omega+i\eta$, where η is a positive infinitesimal. Then the only imaginary part of (4.1) is

$$\mathrm{Im}D(k)=-\pi\delta(\omega-\epsilon_k). \quad (4.4)$$

Therefore

$$\mathrm{Im}A_1\approx(1-\langle n\rangle)(\rho^2V^4/\epsilon_d^2)\ln|\omega/\epsilon_F|, \quad (4.5)$$

where the only approximation involved is that of extracting the leading term for small ω. We note that only small values of ϵ_k and $\epsilon_{k'}$ are involved in producing this Kondo-effect term, as in Kondo's calculation.[3] Terms which are slowly varying for ω, ϵ_k, $\epsilon_{k'}\approx 0$ are not important. Therefore in A_2, we may set $D(\bar{k}''kd)\approx-1/\epsilon_d$, since it is slowly varying for the "sensitive" values of its arguments, while other terms, such as $D(k)$ and the thermal averages give rapidly varying contributions.

Using this approximation and (3.23),

$$A_2 \approx \frac{1}{2\pi}(1-\langle n\rangle)\frac{1}{(-\epsilon_d^2)} \times \sum_{kk''} |V_{kd}|^2 |V_{k''d}|^2 D(k)\frac{n_k - n_{k''}}{\epsilon_k - \epsilon_{k''}} = \tfrac{1}{2}A_1. \quad (4.6)$$

Examining A_3, we see that only one term, $[D(k)+D(k')]$ is rapidly varying in the critical region (the thermal average is small and slowly varying). Therefore A_3 does not contain a $\ln\omega$ term, and is negligible compared to A_1 and A_2.

A_4 is a second-order term, and makes no anomalous contribution.

In A_5, the leading terms in the summand are $D(k)$ and

$$[V_{k'd}D(k')G^{(0)}(d_+) - G^{(1)}(\bar{d}_- k'_- d_+)] \approx -(1/\pi)(1-\langle n\rangle)(V_{k'd}/\epsilon_d)D(k'). \quad (4.7)$$

Substituting,

$$A_5 = (1/\pi\epsilon_d^2)(1-\langle n\rangle) \times \sum_{kk'} |V_{kd}|^2 |V_{k'd}|^2 (1+n_k)D(k)D(k'). \quad (4.8)$$

In this term, there are two imaginary contributions since both the k and k' sums are singular. The presence of the n_k term causes the real part of the k sum (the principal value) to have a $\ln\omega$ dependence, which is absent from the k' sum. The leading term is thus

$$\mathrm{Im}A_5 \approx (1/\pi\epsilon_d^2)(1-\langle n\rangle) \times [\mathrm{Im}\sum_{k'} |V_{k'd}|^2 D(k')][\mathrm{Re}\sum_{k} |V_{kd}|^2 n_k D(k)] = (1-\langle n\rangle)(\rho^2 V^4/\epsilon_d^2)\ln|\omega/\epsilon_F|, \quad (4.9)$$

which is identical to $\mathrm{Im}A_1$.

The contribution A_6 requires special consideration. Its summand contains the product $D(k)G^{(1)}(\bar{d}_- k_- d_+)$ which is proportional to $[D(k)]^2$. However we can show through simple algebra that the factor

$$D(\bar{k}''kd)+D(\bar{d}kk'') = 2D(\bar{k}''kd)D(\bar{d}kk'')[D(k)]^{-1}. \quad (4.10)$$

Therefore the entire summand contains only a single $D(k)$ singularity in the region of interest, and the sum gives no $\ln\omega$ term. If we had replaced the D's on the left of (4.10) by their Fermi-surface values, we would have obtained $A_6=0$, but this would have been an incorrect oversimplification.

In A_7, we set $D(\bar{d}kk')\approx 1/\epsilon_d$, and find that

$$A_7 = \tfrac{1}{2}A_5, \quad (4.11)$$

and therefore gives a $\ln\omega$ contribution.

In the summand for A_8, the function $F(k_+)$ defined in (2.21) appears. Substituting (3.10) in (2.21) yields

$$F(k_+) = \frac{V_{kd}}{2\pi}(1-\langle n_-\rangle)\frac{1-n_k}{\epsilon_d - \epsilon_k}D(d), \quad (4.12)$$

so that $F(k_+)$ is not singular when its arguments are near the Fermi surface. The rest of the integrand has no singularity in this region either because of (4.10). Therefore A_8 is negligible.

The summand for A_9 looks as if it may be singular enough to yield an imaginary $\ln\omega$ term. However, if we note that

$$D(\bar{d}kk')D(k) = [D(k) - D(\bar{d}kk')]/(\epsilon_d - \epsilon_{k'}), \quad (4.13)$$

and, from (4.12), that $F(k'_+) \propto (1-n_{k'})$, we see that it does not.

Summing up, the leading contributions to the imaginary part of $G^{(4)}(d_+)$ are

$$\mathrm{Im}G^{(4)}(d_+) = -(1/\epsilon_d)\mathrm{Im}(A_1+A_2+A_5+A_7) + (\text{second-order terms}). \quad (4.14)$$

Since we are not performing a self-consistent solution for $\langle n_\sigma\rangle$, we will use the lowest order value $\langle n\rangle = \frac{1}{2}$. Then taking the second-order terms from I and the leading fourth-order terms from the preceding calculations in this section, we obtain

$$\mathrm{Im}G^{(4)}(d_+) = -(\rho V^2/2\epsilon_d^2) \times [1+(3\rho V^2/\epsilon_d)\ln|\omega/\epsilon_F|]. \quad (4.15)$$

This is the zero-temperature result. At finite temperatures, $\ln|\omega/\epsilon_F|$ is replaced by

$$\int_{-\epsilon_F}^{\epsilon_F} \frac{f(\epsilon)d\epsilon}{\epsilon-\omega}, \quad (4.16)$$

where $f(\epsilon)$ is the Fermi function, an integral which cannot be expressed as an elementary function.

From (4.15) and (3.5), we obtain for the imaginary part of the band-electron self-energy

$$\mathrm{Im}\,\Sigma_k(\omega) = -(\pi\rho V^4/\epsilon_d^2) \times [1+(3\rho V^2/\epsilon_d)\ln|\omega/\epsilon_F|]. \quad (4.17)$$

The scattering rate for band electrons may be computed from the Schrieffer-Wolff transformation of the Anderson Hamiltonian, which contains ordinary and exchange scattering terms, plus terms which change the d-state occupation by two electrons, and should be negligible according to the authors.[4] If the coefficients in the former two terms are treated as constants (evaluated at the Fermi surface and in the large-U limit), the ordinary term may be easily treated in the first Born approximation, and Kondo's calculation[3] may be used for the exchange term (evaluating his k sums for the square density of states under consideration). (One must note

that the J defined in Ref. 3 equals half the J defined in Ref. 4.) Carrying this out, and noting that the relaxation time τ_k is related to the self-energy by $1/2\tau_k = -\mathrm{Im}\Sigma_k(\epsilon_k)$,[15] we reproduce (4.17) exactly.

5. CONCLUSIONS

Finding a manifestation of the Kondo effect in $G(d_+)$ for the Anderson model comes as no real surprise. The coefficient found for the singular term provides independent confirmation of the arguments given by Schrieffer and Wolff to establish that their transformation extracts the leading term contributing to anomalous scattering.[4]

Our chief goal in carrying out this calculation was to lay firm foundations for a solution of the Anderson model valid below the critical temperature T_c of the Kondo model. The importance of this arises from the fact that the Anderson model preserves the symmetry between the electron producing the local spin and the electron presumed to be bound to it at low temperatures.[5,9] One can expect to gain a qualitative understanding of the behavior of dilute alloys at these temperatures only through such a model.

Several conclusions may be drawn immediately from the present calculation. First, it is clear that no single "path" down the hierarchy of equations of motion is alone responsible for the Kondo effect. There are a great many contributions from various Green's functions; very little of Fig. 4 can be deleted if all the leading V^4 terms are to be retained. Second, we have shown that off-diagonal thermal averages such as $\langle \bar{k}''\_\bar{d}\_+d\_k\_+\rangle^{(2)}$ contribute exactly half of the Kondo anomaly, through expressions such as

$$\sum_{k'} \frac{n_k - n_{k''}}{\epsilon_k - \epsilon_{k''}}, \tag{5.1}$$

while diagonal averages $\langle \bar{k}_\pm k_\pm\rangle^{(0)}$ contribute the other half through

$$\sum_{k'} \frac{n_k}{\omega - \epsilon_k}. \tag{5.2}$$

This is an exact parallel with Nagaoka's high-temperature solution of the Kondo model (see his *Note added in proof*).[5] Third, we point out that a solution valid below T_c may be possible without introducing any further equations of motion than those used here. This conjecture is supported by comparison with Nagaoka's work, since his equations of motion are carried through only to order J^2, which corresponds to our V^4. Such a solution, of course, would be based on a carefully considered *decoupling* approximation rather than the strict-expansion procedure used here. The latter should provide both a motivation for and a check of the former. Fourth, this calculation supports the interpretation of tunneling anomalies given by Appelbaum[16] and Anderson.[17] It does this by verifying the logarithmic peak in the density of states of the impurity-plus-nearer-metal combination, which can be used in an ordinary tunneling formula.[17] It also supports the utility of Anderson's derivation[17] of Appelbaum's Hamiltonian,[16] which is performed by applying the Schrieffer-Wolff transformation[4] to a generalized form of (2.1), by demonstrating the correctness of the tranformation in describing Kondo scattering.

The problem of a self-consistent solution in an applied magnetic field, and hence calculation of the susceptibility, should be deferred until the complete solution in the absence of a field is understood. As we saw in I, such a solution costs V^2 in accuracy, so that a V^6 "strict-expansion" calculation would have been necessary to obtain the proper V^4 correction to the susceptibility.

Note added in proof. In evaluating the various terms in $G(d_+)$, attention was focused on contributions to the various k integrals from near the Fermi surface. It has come to the author's attention that anomalous contributions can arise from certain of the terms when one ϵ_k is near ϵ_d. In these terms, energy denominators such as $D(\bar{d}kk')$ were heretofore approximated as ϵ_d^{-1}. Keeping the contributions $-i\pi\delta(\omega+\epsilon_d-\epsilon_k-\epsilon_{k'})$ from such denominators gives additional imaginary log terms of the order kept. However, all such additional contributions cancel, leaving the result unchanged. Inclusion of these terms does re-arrange the sources of the Kondo scattering. The total singular contribution of each of the terms A_2 and A_7 goes to zero, and A_8 makes a compensating contribution. Other individual terms are unchanged.

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