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Thermodynamic scaling theory for impurities in metals

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A perturbative scaling theory for calculating static thermodynamic properties of arbitrary *local* impurity degrees of freedom interacting with the conduction electrons of a metal is presented. The basic features are developments of the ideas of Anderson and Wilson, but the precise formulation is new and is capable of taking into account band-edge effects which cannot be neglected in certain problems. Recursion relations are derived for arbitrary interaction Hamiltonians up to third order in perturbation theory. A generalized impurity Hamiltonian is defined and its scaling equations are derived up to third order. The strategy of using such perturbative scaling equations is delineated and the renormalization-group aspects are discussed. The method is illustrated by applying it to the single-impurity Kondo problem whose static properties are well understood.

I. INTRODUCTION

A variety of many-body problems of current interest involves conduction electrons of a metal interacting with *localized* "impurity" degrees of freedom that can be represented by a finite number of discrete "impurity" states. Examples of such problems are the following: a small number of magnetic impurities in a nonmagnetic metal,[1] the x-ray absorption and emission problems where a core hole interacts with the conduction electrons in a metal,[2] the interaction of conduction electrons with the tunneling states in a metallic glass,[3] and the interaction between conduction electrons and atoms chemisorbed on metallic surfaces.[4]

The Hamiltonians that are normally used to model the above problems have the following structure, which will be called the "generalized impurity Hamiltonian,"

$$\mathscr{H}=\mathscr{H}_0+\mathscr{U}+\int_{\epsilon,\mu}[\mathscr{V}^{\dagger}(\epsilon,\mu)c_{\epsilon\mu}+\text{H.c.}] + \int_{\epsilon,\mu}\int_{\epsilon',\mu'}c^{\dagger}_{\epsilon\mu}\mathscr{S}(\epsilon,\mu;\epsilon',\mu')c_{\epsilon'\mu'}+\cdots \quad (1.1)$$

Here $\mathscr{H}_0$ represents the conduction band of the metal, $c^{\dagger}_{\epsilon\mu}$ is the creation operator for a conduction electron of energy ϵ (measured from the Fermi level) with μ labeling all its other attributes such as spin, angular momentum, etc., and $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$ are *operators* in the space of impurity states. If the impurity states and the operators $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$ are nontrivial, successive scatterings of conduction electrons from the impurity become correlated, leading to a coupling of the various conduction-electron energy scales in the problem. This renders the calculation of the properties nontrivial, and exact results are known only in rather special cases. In particular, perturbation theory in $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$ is plagued by the divergence difficulties typified by the logarithmic divergences encountered in the Kondo problem.[5]

In an attempt to handle these divergences, Anderson, in a pioneering paper in 1970,[6(a)] formulated a perturbative scaling method for the Kondo problem, which, however, provided only a qualitative solution. A quantitative solution was obtained by Wilson, who, in addition to developing the general conceptual framework of the renormalization-group (RG) formalism[7] for critical phenomena and quantum field theory, devised a powerful, nonperturbative, numerical RG technique for the Kondo problem.[8] In this paper we present a new, thermodynamic formulation[9] of perturbative scaling that attempts to generalize, and render more precise, Anderson's method in the light of the insights provided by Wilson's work, so that it is applicable to a broad class of problems involving impurities in metals.

The basic scheme of the scaling method presented in this paper is as follows: Let D_0 be the band edge or the cutoff of the conduction-electron spectrum in $\mathscr{H}_0$. One "eliminates" the higher (i.e., near the cutoff) energy scales in the problem so as to reduce the cutoff from D_0 to D, but at the same time one changes the Hamiltonian from $\mathscr{H}_0+\mathscr{H}_I$ to $\mathscr{H}_0+\mathscr{H}_I(D)$ so as to preserve the low-temperature properties of the problem. Specifically, divide the eigenstates of $\mathscr{H}_0$ into a set $\{|p\rangle\}$ that contains no electrons or holes of energy $D<\epsilon<D_0$ and a complementary set $\{|q\rangle\}$ that contains *at least one* electron or hole of energy $D<\epsilon<D_0$. Clearly $E_0(q)$, the energy of the state $|q\rangle$, is larger than D. Now consider the evaluation of $\text{Tr}\exp[-\beta(\mathscr{H}_0+\mathscr{H}_I)]$ by perturbation theory in $\mathscr{H}_I$, and systematically neglect terms of order $e^{-\beta E_0(q)}$, since typically one is interested in temperatures $T \ll D < D_0$. Then one can show that the remaining terms in the perturbation correspond to evaluating $\text{Tr}\exp\{-\beta[\mathscr{H}_0+\mathscr{H}_I(D)]\}$, where the trace is now taken only over the states $\{|p\rangle\}$.[10] In this paper the recursion relation between $\mathscr{H}_I$ and $\mathscr{H}_I(D)$ is developed up to third order in $\mathscr{H}_I$.

The above procedure, which essentially permits one to define a renormalization-group transformation (RGT), can be applied to the generalized impurity Hamiltonian defined by (1.1). The new Hamiltonian $\mathscr{H}_0+\mathscr{H}_I(D)$ with cutoff D can also be represented in the form (1.1), but is different from the old Hamiltonian $\mathscr{H}_0+\mathscr{H}_I$ with cutoff D_0 in two ways: (1) It has altered "values" $\mathscr{U}_D$, $\mathscr{V}_D$, and $\mathscr{S}_D$ of the couplings $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$. (2) It has *new* forms of local coupling between the impurity and the conduction electrons, corresponding to two-electron scattering, three-electron scattering, etc.; but these new couplings can be shown to be irrelevant in the RG sense, and hence can be neglected for many purposes. One can therefore represent the recursion relation between $\mathscr{H}_I(D)$ and $\mathscr{H}_I$ in terms of recursion relations between $\mathscr{U}_D$, $\mathscr{V}_D$, and $\mathscr{S}_D$ and $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$, and explicit algebraic expressions for these recursions are worked out up to third order in $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$.

The scaling method and the above "generalized" recursion relations can be of great value in studying various impurity-type problems. Setting up and solving such recursion relations for the coupling constants in any specific problem enables one to improve upon naive perturbation theory considerably and is equivalent to summing up specific infinite subsets of terms in perturbation theory.[11] We illustrate this using the familiar single-impurity Kondo problem, where the impurity is a spin-$\frac{1}{2}$ degree of freedom $\vec{S}$ and $\mathscr{H}_I=-(J_0/2)\vec{S}\cdot\vec{s}(0)$, where $\vec{s}_0$ represents the conduction-electron spin density at the impurity site. In particular, it is shown that the dominant interaction in $\mathscr{H}_I(D)$ is of the form $-(J_D/2)\vec{S}\cdot\vec{s}(0)$, and that by neglecting terms of the order of (T/D) and (D/D_0), $J(D)$ satisfies the recursion relation

$$\frac{d(\rho_0 J)}{d\ln(D/D_0)}=(\rho_0 J)^2+\tfrac{1}{2}(\rho_0 J)^3+\cdots\ , \tag{1.2}$$

in agreement with earlier results.[9(a)] There are many subtle aspects associated with the use of scaling methods in general, and with the derivation of recursion relations such as (1.2) in particular. These are also discussed in the context of the Kondo problem for pedagogical reasons.

It is worthwhile stressing the following important feature of our scaling method. It is a thermodynamic scaling theory: The main approximation is the neglect of terms of order $e^{-(D/T)}$, and we are able to keep track of coupling terms that determine the energy dependence of $\mathscr{V}$ and $\mathscr{S}$, whose contribution to the thermodynamics is of order (T/D_0), whereas earlier scaling theories neglected these terms. Such terms can be shown to constitute irrelevant operators in the RG sense, but they can be crucially important in some problems where they are accompanied by large coefficients. For example, consider the two-impurity Kondo problem with a model Hamiltonian in which two impurity spins $\vec{S}_1$ and $\vec{S}_2$, separated by a distance R, each interact with the conduction electrons via the Kondo coupling. One can show that the recursion procedure developed in this paper generates an interaction of the form $I(R)\vec{S}_1\cdot\vec{S}_2$, where $I(R)$ is the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction.[12] However, the correct oscillatory dependence of $I(R)$ on R can be reproduced only if the above-mentioned irrelevant operators determining the energy dependence of (RD/V_F) are kept track of properly. The reason is that in the two-impurity Kondo problem the irrelevant operators are accompanied by large coefficients of the order of (RD/V_F), and must be included at least in the initial stages of the recursions. This can be done in our formulation of the scaling procedure, in contrast to previous methods.[13]

The basic strategy of the scaling method would be to carry out the scaling until $D\simeq 10T$ (since the main approximation of neglecting terms of order $e^{-D/T}$ is still good at $D\simeq 10T$), and to calculate properties with the final Hamiltonian thereby obtained, to be denoted $\mathscr{H}_{\text{eff}}(T)$. The usefulness of this idea stems from the expectation[14] that the sequence of scaled Hamiltonians, i.e., the trajectory of $\mathscr{H}_{\text{eff}}(T)$ as a function of decreasing T in the space of generalized impurity Hamiltonians, will often be in the form of a crossover from the vicinity of one fixed point of the RGT to that of another. In other words, the full range of $T<D_0$ breaks up into various regimes in each of which $\mathscr{H}_{\text{eff}}(T)$ is close to some fixed point, whence the relevant and marginal deviations of $\mathscr{H}_{\text{eff}}(T)$ from the fixed point constitute small parameters in the problem. Perturbation theory in these small parameters is necessarily divergence free as the effective cutoff in $\mathscr{H}_{\text{eff}}(T)$ is $10T$ by construction. The important point is that one can trace the trajectory of $\mathscr{H}_{\text{eff}}(T)$ within each such "regime of a fixed point"[15] quite well using the perturbative scaling techniques, in terms of some undetermined parameters. Of course, in order to relate these parameters to the initial coupling constants in the model Hamiltonian in any given problem, one must be able to calculate the trajectory of $\mathscr{H}_{\text{eff}}(T)$ through its crossover from one fixed point to another. While this can occasionally be done reasonably well using the perturbative scaling methods, in general[16] it needs the use of nonperturbative, numerical RG techniques of the type developed by Wilson. But even in such cases it often will be necessary to use our perturbative recursion relations in the preliminary stages of scaling, and thereby obtain the input Hamiltonians to be fed into the numerical RGT: This is especially true if irrelevant operators with large coefficients are present in the initial model Hamiltonian, as typified by the two-impurity Kondo problem.

The rest of this paper is organized as follows: The generalized impurity Hamiltonian is defined and illustrated with examples in Sec. II. Section III is devoted to the formal development of our scaling method, where the recursion relations between $\mathscr{H}_I(D)$ and $\mathscr{H}_I(D_0)$ are obtained. These results are applied to the generalized impurity Hamiltonian in Sec. IV, and their renormalization-group aspects are brought out in Sec. V. Section VI is devoted to the illustration of the usefulness of the scaling methods using the single-impurity Kondo problem as an example. Section VII contains some concluding remarks. The Appendixes contain various technical details.

II. THE GENERALIZED IMPURITY PROBLEM

For simplicity it will be assumed in this paper that the conduction band of the metal is isotropic with some density of states $\rho_0(\epsilon)$ between $\pm D_0$ about the Fermi level. It is then convenient to label the conduction-electron creation operators using the energy representation as $c^\dagger_{\epsilon\mu}$, where, depending on the problem, μ stands for other *discrete or continuous* labels of the electron. For example, $\mu\equiv(\hat{k},\alpha)$ where $\hat{k}$ is the direction of the wave vector of the electron and α is its spin, or $\mu\equiv(m_z\alpha)$ where m_z is the z component of the angular momentum of the electron, and so on. [Actually, by letting the density of states $\rho_0(\epsilon)$ depend upon an appropriately defined μ, more general band structures might be represented.] In this representation the conduction-band Hamiltonian takes the form

$$\mathscr{H}_0=\int_{\epsilon\mu}\epsilon c^\dagger_{\epsilon\mu}c_{\epsilon\mu} \ , \tag{2.1}$$

where $\int_{\epsilon,\mu}$ stands for $\sum_\mu\int d\epsilon\rho_0(\epsilon)$, the electron operators obey the anticommutation relations

$$\{c^\dagger_{\epsilon\mu},c_{\epsilon'\mu'}\}=\delta_{\mu\mu'}\delta(\epsilon-\epsilon')/\rho_0(\epsilon) \ , \tag{2.2}$$

and $\sum_\mu$ and $\delta_{\mu\mu'}$ have appropriate discrete and continuum meanings depending upon the context. With the use of this same representation, the generalized impurity Hamiltonian introduced in Sec. I can be written as

$$\mathscr{H}=\mathscr{H}_0+\mathscr{H}_I=\mathscr{H}_0+\mathscr{H}_{I1}+\mathscr{H}_{I2}+\mathscr{H}_{I3}+\cdots \ , \tag{2.3a}$$

$$\mathscr{H}_{I1}=\mathscr{U} \ , \tag{2.3b}$$

$$\mathscr{H}_{I2}=\int_{\epsilon,\mu}[\mathscr{V}^\dagger(\epsilon,\mu)c_{\epsilon\mu}+c^\dagger_{\epsilon\mu}\mathscr{V}(\epsilon,\mu)] \ , \tag{2.3c}$$

$$\mathscr{H}_{I3}=\int_{\epsilon,\mu}\int_{\epsilon',\mu'}c^\dagger_{\epsilon\mu}c_{\epsilon'\mu'}\mathscr{S}(\epsilon,\mu;\epsilon',\mu') \ , \tag{2.3d}$$

where $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$ are *operators* in the finite-dimensional space of the impurity states, and where $\mathscr{U}$ and $\mathscr{S}$ commute but $\mathscr{V}$ anticommutes with $c_{\epsilon\mu}$ and $c^\dagger_{\epsilon\mu}$. Clearly, $\mathscr{H}_{I1}$ represents intra-impurity energy-splitting terms, $\mathscr{H}_{I2}$, one-electron mixing terms, and $\mathscr{H}_{I3}$, one-electron scattering terms. It is worthwhile illustrating the use of (2.3) with some examples.

A. Single-impurity isotropic Kondo problem

Here a spin-$\frac{1}{2}$ impurity $\vec{S}$ interacts only with the s-wave conduction electron localized around it via the Hamiltonian

$$\begin{aligned}\mathscr{H}_I&=J_0\vec{S}\cdot\vec{s}(0)\\&=-\frac{J_0}{2}\int_{\epsilon,\alpha}\int_{\epsilon',\alpha'}c^\dagger_{\epsilon\alpha}\vec{\sigma}_{\alpha\alpha'}C_{\epsilon'\alpha'}\cdot\vec{S} \ .\end{aligned} \tag{2.4a}$$

In this case μ need stand only for the spin label, and it is easy to see that (2.4a) is of the form (2.3) with $\mathscr{U}$ and $\mathscr{V}$ zero and

$$\mathscr{S}(\epsilon,\alpha;\epsilon',\alpha')=-\frac{J_0}{2}\vec{S}\cdot\vec{\sigma}_{\alpha\alpha'} \ . \tag{2.4b}$$

To include potential scattering and permit anisotropic exchange interaction one would merely have to write

$$\begin{aligned}\mathscr{S}(\epsilon,\alpha;\epsilon',\alpha')=K_0\delta_{\alpha\alpha'}&-\frac{J_z}{2}S^z\sigma^z_{\alpha\alpha'}\\&-\frac{J_1}{2}(S^x\sigma^x_{\alpha\alpha'}+S^y\sigma^y_{\alpha\alpha'}) \ ,\end{aligned} \tag{2.4c}$$

whereas the presence of a local magnetic field acting on the impurity alone could be accommodated by adding $-g\mu_B HS_z$ to $\mathscr{U}$.

B. Nondegenerate (s-wave) Anderson model (Ref. 17)

Here the impurity is represented by an orbital degree of freedom with four states, and one has $\mathscr{S}=0$ and

$$\mathscr{U}=\epsilon_d\sum_\sigma n_{d\sigma}+Un_{d+}n_{d-} \ , \tag{2.5a}$$

$$\mathscr{V}(\epsilon,\alpha)=V_d c_{d\alpha} \ . \tag{2.5b}$$

If one wants to consider more realistic models of magnetic impurities in metals, such as the degenerate Anderson or Hirst models,[18] one can extend μ to include angular momentum or crystal-field channel labels, and $\mathscr{U}$ to include intra-impurity Coulomb energies, Hund's-rule couplings, LS term, crystal-field and spin-orbit splittings, etc.

C. The two-impurity Kondo problem

Here one has two spins $\vec{S}_1$ and $\vec{S}_2$ situated at $(0,0,\pm R/2)$, each interacting with the conduction electrons via the isotropic Kondo exchange scattering, i.e.,

$$\begin{aligned}\mathscr{H}=\mathscr{H}_0-\frac{J_0}{2}\Bigg[&\psi^\dagger_\alpha\left(\frac{R}{2}\right)\vec{\sigma}_{\alpha\alpha'}\psi_{\alpha'}\left(\frac{R}{2}\right)\cdot\vec{S}_1\\&+\psi^\dagger_\alpha\left(-\frac{R}{2}\right)\vec{\sigma}_{\alpha\alpha'}\psi_{\alpha'}\left(-\frac{R}{2}\right)\cdot\vec{S}_2\Bigg] \ ,\end{aligned} \tag{2.6a}$$

where the $\psi_\alpha(\pm R/2)$'s represent the conduction-electron annihilation operators localized at the impurity sites. For concreteness assume that the conduction-electron wave functions are plane waves labeled by $\vec{k}\equiv(k_\epsilon,\hat{k})$. In this case it is enough to let $\mu\equiv(\zeta,\alpha)$, where α is the spin index and $\zeta=\cos\theta$, with θ the polar angle of $\vec{k}$ relative to the axis passing through the impurity positions; and one has $\mathscr{U}$ and $\mathscr{V}$ zero and

$$\mathscr{S}(\epsilon,\zeta,\alpha;\epsilon',\zeta',\alpha')=-\frac{J_0}{2}(e^{-iQ(R/2)}\vec{S}_1+e^{iQ(R/2)}\vec{S}_2)\cdot\vec{\sigma}_{\alpha\alpha'}$$

with

$$Q=(k_\epsilon\zeta-k_{\epsilon'}\zeta') \ . \tag{2.6b}$$

Note that the energy dependence of $\mathscr{S}$ is quite crucial in this case and has all the information that one needs here in a two-impurity problem.

D. X-ray absorption and emission problems in metals (Ref. 19)

In the simplest of the models representing this process one neglects the finite lifetime of the core hole, dynamical screening processes, etc., and models the core hole by a deep two-state (occupied and unoccupied) level interacting with spinless s-wave conduction electrons. In this case the label m is unnecessary and $d^\dagger$ is the creation operator for filling the core hole. A screened contact potential interaction between the core hole and the conduction electrons is represented by $\mathscr{S}(\epsilon,\epsilon')=Gdd^\dagger$ and by the energy of the core state of the form of $\mathscr{U}=\epsilon_d d^\dagger d$. The Hamiltonian is easily modified, but still keeping it within the framework of the generalized impurity problem, to include various complications, such as realistic band structures, momentum-dependent interactions between the core hole and the conduction electrons, coupling to other angular-momentum channels, etc.

For later use it is convenient to normal order the Hamiltonian (2.3); i.e., to remember that the negative-energy electron states are occupied in the ground state and that the low-lying excited states correspond to the presence of a few holes, and hence to represent (2.3) in terms of positive-energy electron and hole operators. Letting $b^\dagger_{\epsilon\mu}\equiv c_{-\epsilon\mu}$ represent the creation operator for a hole of energy ϵ and $a^\dagger_{\epsilon\mu}\equiv c^\dagger_{\epsilon\mu}$ the creation operator for an electron of energy ϵ, one gets

$$\mathscr{H}_0=\int_{\epsilon,\mu}\epsilon(a^\dagger_{\epsilon\mu}a_{\epsilon\mu}+b^\dagger_{\epsilon\mu}b_{\epsilon\mu})\;, \tag{2.7a}$$

$$\mathscr{H}_I=\mathscr{H}_{I1}+\mathscr{H}_{I2}+\mathscr{H}_{I3}\;, \tag{2.7b}$$

$$\mathscr{H}_{I1}=\mathscr{U}\;, \tag{2.7c}$$

$$\mathscr{H}_{I2}=\int_{\epsilon\mu}\{[\mathscr{V}^\dagger(\epsilon,\mu)a_{\epsilon\mu}+\mathscr{V}(-\epsilon,\mu)b^\dagger_{\epsilon\mu}]+\text{H.c.}\} \tag{2.7d}$$

$$\begin{aligned}\mathscr{H}_{I3}=\int_{\epsilon,\mu}\int_{\epsilon',\mu'}&[a^\dagger_{\epsilon\mu}a_{\epsilon'\mu'}\mathscr{S}(\epsilon,\mu;\epsilon',\mu')+b_{\epsilon\mu}a_{\epsilon\mu}\mathscr{S}(-\epsilon,\mu;\epsilon',\mu')\\&+a^\dagger_{\epsilon\mu}b^\dagger_{\epsilon'\mu'}\mathscr{S}(\epsilon,\mu;-\epsilon',\mu')-b^\dagger_{\epsilon\mu}b_{\epsilon'\mu'}\mathscr{S}(-\epsilon',\mu';-\epsilon,\mu)]\;.\end{aligned} \tag{2.7e}$$

In this case $\int_{\epsilon,\mu}$ stands for $\sum_\mu\int_0^{D_0}d\epsilon\rho_0(\pm\epsilon)$, depending on whether electron or hole degrees of freedom are being considered. In writing (2.7) all constant (ground-state energy) terms have been ignored, and the term $\int_{\epsilon,\mu}\mathscr{S}(-\epsilon,\mu;-\epsilon,\mu)$ that comes from normal ordering (2.3d) is considered to be included in $\mathscr{U}$. Hereafter, whenever any reference to the generalized impurity Hamiltonian is made, the normal-ordered form (2.7) will be meant.

III. THE THERMODYNAMIC SCALING METHOD—FORMAL DEVELOPMENT

In this paper we will discuss only the calculation of static properties. Then without loss of generality one can focus on the calculation of the partition function

$$Z\equiv\text{Tr}\,e^{-\beta\mathscr{H}}=\text{Tr}\,e^{-\beta(\mathscr{H}_0+\mathscr{H}_I)}\;. \tag{3.1}$$

This is sufficient since any static property involves the calculation of $\text{Tr}(Ae^{-\beta\mathscr{H}})$, where A is some operator, and this can be obtained from $\text{Tr}\,e^{-\beta(\mathscr{H}+hA)}$ where $\mathscr{H}+hA$ can itself be considered to be another generalized impurity Hamiltonian.

As emphasized in the Introduction this can be a difficult many-body problem in the case of impurities with nontrivial $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$. In particular, even perturbative calculations are plagued by divergence difficulties. These divergences arise from the fact that for nontrivial $\mathscr{V}$ and $\mathscr{S}$ successive scatterings of conduction electrons by the impurity get correlated, leading to a coupling of the various conduction-electron energy scales in the problem.[8] To see this, note that because of the Boltzmann factor $e^{-\beta\mathscr{H}}$ in Z, levels of $\mathscr{H}$ with energy much greater than k_BT above the ground state do not contribute, and energy levels which are split on a much finer scale than k_BT get smeared over. Hence, roughly speaking, it is the difference between the energy-level structure of $\mathscr{H}$ and of $\mathscr{H}_0$ on the scale of k_BT that determines Z/Z_0. In perturbative calculations of this structure states containing electron or hole excitations of energy $D_0>\epsilon\gg k_BT$ can come in only as virtual states, but can thereby give rise to logarithmic divergences via energy integrals such as

$$\int_{k_BT}^{D_0}\frac{d\epsilon}{\epsilon}\sim\ln\left[\frac{D_0}{k_BT}\right]\;, \tag{3.2}$$

since such integrals become large for $D_0\gg k_BT$. Thus the divergences are due to the presence of coupled conduction-electron and hole excitations of energy between k_BT, the energy scale of interest, and D_0, the cutoff energy scale. They are similar to the divergences encountered in critical phenomena and quantum field theory.[7]

The scaling or the renormalization-group transformation (RGT) is a recursive procedure to "eliminate" or "integrate out" the higher (i.e., near the cutoff) energy scales in the problem so as to reduce the cutoff from D_0 to a new value $D<D_0$, but in such a way as to preserve the structure of the energy-level splitting of the Hamiltonian on the scale of k_BT. Our prescription to define this recursive procedure is as follows: Consider evaluating Z given by (3.1) treating $\mathscr{H}_I$ in perturbation theory. The various terms that result involve [see Eqs. (3.3a)—(3.3d)] sums over eigenstates of $\mathscr{H}_0$ as intermediate states, weighted by appropriate Boltzmann factors. Now divide the set of eigenstates of $\mathscr{H}_0$ into a set $\{\,|p\rangle\}$, which contains *no electron or hole excitations* of energy $D>\epsilon>D_0$, and a complementary set $\{\,|q\rangle\}$ (the two sets together span the Hilbert space), which contains *at least one* electron or hole of energy $D<\epsilon<D_0$. Since $E_q\geq D$ and $k_BT\ll D$, one can systematically neglect[20] terms in the

perturbation series of the order of $e^{-\beta E_q}$ while making errors only of order $e^{-D/T}$. It is shown below that, *order by order in perturbation theory,* one can find a Hamiltonian $\mathcal{H}_I(D)$ such that the remaining terms in the perturbation series are equal to $\mathrm{Tr}_P e^{-\beta[\mathcal{H}_0+\mathcal{H}_I(D)]}$, where the trace symbolized by Tr_P is taken only over the set $\{\,|p\rangle\}$. The relation between $\mathcal{H}_I(D)$ and $\mathcal{H}_I$ up to third order in $\mathcal{H}_I$ is given by

$$\mathcal{H}_I(D)=\mathcal{H}_I^{(1)}(D)+\mathcal{H}_I^{(2)}(D)+\mathcal{H}_I^{(3)}(D)+\cdots\ , \tag{3.3a}$$

$$\mathcal{H}_I^{(1)}(D)=P\mathcal{H}_I P\ , \tag{3.3b}$$

$$\mathcal{H}_I^{(2)}(D)=-\tfrac{1}{2}\sum_{a,b,q} P_a\mathcal{H}_I\,|q\rangle\langle q\,|\mathcal{H}_I P_b\left[\frac{1-e^{-\beta(E_q-E_a)}}{E_q-E_a}+\frac{1-e^{-\beta(E_q-E_b)}}{E_q-E_b}\right], \tag{3.3c}$$

$$\mathcal{H}_I^{(3)}(D)=\tfrac{1}{4}(\mathcal{P}_I^{[\mathrm{I}]}+\mathcal{P}_I^{[\mathrm{II}]}\ ,$$

with

$$\mathcal{P}_I^{[\mathrm{I}]}=\sum_{a,b,q_1,q_2} P_a\mathcal{H}_I\,|q_1\rangle\langle q_1|\,\mathcal{H}_I\,|q_2\rangle\langle q_2\,|\mathcal{H}_I P_b\left[\frac{1-e^{-\beta(E_{q_1}-E_a)}}{E_{q_1}-E_a}+\frac{1-e^{-\beta(E_{q_1}-E_b)}}{E_{q_1}-E_b}\right]$$
$$\times\left[\frac{1-e^{-\beta(E_{q_2}-E_a)}}{E_{q_2}-E_a}+\frac{1-e^{-\beta(E_{q_2}-E_b)}}{E_{q_2}-E_b}\right] \tag{3.3d}$$

and

$$\mathcal{P}_I^{[\mathrm{II}]}=\sum_{a,b,p,q}(P_a\mathcal{H}_I\,|p\rangle\langle p\,|\mathcal{H}_I\,|q\rangle\langle q\,|\mathcal{H}_I P_b+\mathrm{H.c.})\left[\frac{1-e^{-\beta(E_p-E_a)}}{E_p-E_a}+\frac{1-e^{-\beta(E_p-E_b)}}{E_p-E_b}\right]$$
$$\times\left[\frac{1-e^{-\beta(E_q-E_a)}}{E_q-E_a}-\frac{1-e^{-\beta(E_q-E_p)}}{E_q-E_p}\right].$$

Here the notation used signifies that the states $|q\rangle$, $|q_1\rangle, |q_2\rangle$ belong to the set $\{\,|q\rangle\}$ and $|a\rangle$, $|b\rangle, |p\rangle$ belong to the set $\{\,|p\rangle\}$, while E_q, $E_{q_1}, \cdots$ are the energy eigenvalues of $\mathcal{H}_0$ in these states, and P_a, P_b, and P are the projection operators for the subspaces spanned by $|a\rangle$, $|b\rangle$, and the entire set $\{\,|p\rangle\}$, respectively. The recursion relations (3.3a)—(3.3d) are the central results of this section.[21] Before proceeding to their derivation, it is worthwhile commenting on several important features of these relations.

A. Weak temperature dependence

The recursive procedure discussed above transforms the old problem of evaluating $\mathrm{Tr}\, e^{-\beta(\mathcal{H}_0+\mathcal{H}_I)}$ over states with cutoff D_0 into the new problem of evaluating $\mathrm{Tr}_P e^{-\beta[\mathcal{H}_0+\mathcal{H}_I(D)]}$ over states with cutoff $D<D_0$. The new Hamiltonian $\mathcal{H}_0+\mathcal{H}_I(D)$ depends both on D and on the temperature k_BT (strictly speaking D/D_0 and k_BT/D_0), although, as will be seen later, the temperature dependence is weak and can be ignored for many purposes (and hence has been suppressed in the notation). Since the recursions have been derived for a finite reduction in the cutoff, it is trivial to convert them into differential recursions for an infinitesimal change in the cutoff by letting $D\to D_0-\delta D$.

B. Nonsingularity

Although the expressions (3.3c) and (3.3d) involve energy denominators that vanish, the complete expressions are nonsingular and well behaved. The presence of the temperature-dependent terms in (3.3c) and (3.3d) is crucial in ensuring this and is related to the point made earlier, namely, that energy levels split on a scale much smaller than k_BT are smeared over, so that k_BT provides a lower cutoff for energy splittings.

C. Semigroup property

There is some degree of arbitrariness in the choice of $\mathcal{H}_I(D)$, since only the partition function has been required to be preserved (up to terms of order $e^{-D/T}$) by the transformation. Apart from considerations of hermiticity and symmetry, the specific choice given by (3.3a)—(3.3d) has been made such that it ensures the semigroup property of the RGT. Namely, if $D'<D_0$, then the Hamiltonian obtained by a direct transformation reducing the cutoff from D_0 to D' must be the same (up to terms of order $e^{-D'/T}$ and $e^{-D/T}$) as the Hamiltonian obtained from two successive transformations reducing the cutoff first from D_0 to D, and then from D to D'. That the choice (3.3a)—(3.3d) satisfies this requirement is proven in Appendix B, but it must be noted that this requirement still does not uniquely fix the recursions.

D. Ground-state energy terms

Ideally, one might have wished the recursion relations to have the property that if $\mathcal{H}_I \to \mathcal{H}_I + \Delta$ where Δ is a constant, then $\mathcal{H}_I^{(1)}(D) \to \mathcal{H}_I^{(1)} + \Delta$, while $\mathcal{H}_I^{(2)}(D)$, $\mathcal{H}_I^{(3)}(D)$, etc., are unaffected. We have *not* been able to find a way to meet this requirement. In particular, $\mathcal{H}_I^{(3)}(D)$ given by (3.3d) does pick up extra terms, although these terms do not make any contribution to the partition function. It is convenient to avoid such terms by ensuring that *at every stage of the iteration* (3.3) does not contain any constant terms, i.e., ground-state energy terms are always included as part of $\mathcal{H}_0$ and not of $\mathcal{H}_I$.

Next we present the proofs of the various results stated above. For convenience of exposition, only the basic outline will be presented in the text, and the algebra and the technical details will be relegated to the Appendixes.

Consider the perturbation expansion for the partition function (3.1).[22] One can write this as

$$Z = Z^{(0)} + Z^{(1)} + Z^{(2)} + \cdots \,, \tag{3.4a}$$

$$Z^{(0)} = \sum_j e^{-\beta E_j} \,, \tag{3.4b}$$

$$Z^{(1)} = -\beta \sum_j \langle j \,|\, \mathcal{H}_I \,|\, j \rangle e^{-\beta E_j} \,, \tag{3.4c}$$

and the nth-order term (for $n > 1$) is given by

$$Z^{(n)} = -\frac{\beta}{n} \sum_{j_1, \ldots, j_n} \langle j_1 \,|\, \mathcal{H}_I \,|\, j_2 \rangle \cdots \langle j_n \,|\, \mathcal{H}_I \,|\, j_1 \rangle \left[\sum_{m=1}^{n} e^{-\beta E_{j_m}} \prod_{k \neq m} \frac{1}{E_{j_m} - E_{j_k}} \right] . \tag{3.4d}$$

A proof of this result is presented in Appendix A. In the above expressions $|j\rangle$, $|j_1\rangle, \cdots$ denote the eigenstates of $\mathcal{H}_0$ and E_j, $E_{j_1}, \cdots$ denote their energies. Note that the entire expression within the large parentheses in (3.4d) is an analytic function of all the energies E_{j_k}.

Next one makes the division of the eigenstates of $\mathcal{H}_0$ into the sets $\{ |p\rangle \}$ and $\{ |q\rangle \}$ discussed earlier. The subspaces spanned by these sets as well as their projection operators will be denoted P and Q. To any order the term in which all the intermediate states belong to Q is of order $e^{-D/T}$ and can be neglected. The remaining terms up to third order are, using obvious notation,

$$Z^{(0)} \cong \sum_p e^{-\beta E_p} \,, \tag{3.5a}$$

$$Z^{(1)} \cong -\beta \sum_p \langle p \,|\, \mathcal{H}_I \,|\, p \rangle e^{-\beta E_p} \,, \tag{3.5b}$$

$$Z^{(2)} \cong -\frac{\beta}{2} \left[\sum_{p_1, p_2} \langle p_1 \,|\, \mathcal{H}_I \,|\, p_2 \rangle \langle p_2 \,|\, \mathcal{H}_I \,|\, p_1 \rangle \left[\frac{e^{-\beta E_{p_1}} - e^{-\beta E_{p_2}}}{E_{p_1} - E_{p_2}} \right] + 2 \sum_{p,q} \langle p \,|\, \mathcal{H}_I \,|\, q \rangle \langle q \,|\, \mathcal{H}_I \,|\, p \rangle \left[\frac{e^{-\beta E_p} - e^{-\beta E_q}}{E_p - E_q} \right] \right] , \tag{3.5c}$$

$$\begin{aligned} Z^{(3)} \cong -\frac{\beta}{3} \Bigg[& \sum_{p_1, p_2, p_3} \langle p_1 \,|\, \mathcal{H}_I \,|\, p_2 \rangle \langle p_2 \,|\, \mathcal{H}_I \,|\, p_3 \rangle \langle p_3 \,|\, \mathcal{H}_I \,|\, p_1 \rangle \left[\frac{e^{-\beta E_{p_1}}}{(E_{p_1} - E_{p_2})(E_{p_1} - E_{p_3})} + \cdots \right] \\ & + 3 \sum_{p_1, p_2, q} \langle q \,|\, \mathcal{H}_I \,|\, p_1 \rangle \langle p_1 \,|\, \mathcal{H}_I \,|\, p_2 \rangle \langle p_2 \,|\, \mathcal{H}_I \,|\, q \rangle \left[\frac{e^{-\beta E_{p_1}} - e^{-\beta E_q}}{(E_{p_1} - E_q)(E_{p_1} - E_{p_2})} + (p_1 \leftrightarrow p_2) \right] \\ & + 3 \sum_{p, q_1, q_2} \langle p \,|\, \mathcal{H}_I \,|\, q_1 \rangle \langle q_1 \,|\, \mathcal{H}_I \,|\, q_2 \rangle \langle q_2 \,|\, \mathcal{H}_I \,|\, p \rangle \left[\frac{e^{-\beta E_p} - e^{-\beta E_{q_1}}}{(E_p - E_{q_1})(E_{q_1} - E_{q_2})} + (q_1 \leftrightarrow q_2) \right] \Bigg] . \end{aligned}$$

Now consider the question of whether one can find $\mathcal{H}_I(D)$ such that $\mathrm{Tr}_P \exp\{ -\beta[\mathcal{H}_0 + \mathcal{H}_I(D)] \}$ agrees order by order in perturbation theory with the terms in (3.5) (up to terms of order $e^{-D/T}$). Breaking up $\mathcal{H}_I(D)$ into its various orders as in (3.3a), one can write

$$\mathrm{Tr}_P \exp\{ -\beta[\mathcal{H}_0 + \mathcal{H}_I(D)] \} = \mathrm{Tr} \exp\{ -\beta[\mathcal{H}_0 + \mathcal{H}_I^{(1)}(D) + \mathcal{H}_I^{(2)}(D) + \cdots] \} \,. \tag{3.6}$$

Now one can expand the right-hand side using the perturbation expansion (3.4), and compare order by order with (3.5) to obtain various conditions on $\mathcal{H}_I^{(n)}(D)$. The zeroth-order terms evidently agree. Comparing the first-order terms yields the condition

$$-\beta \sum_p \langle p \,|\, \mathcal{H}_I^{(1)} \,|\, p \rangle e^{-\beta E_p} = Z^{(1)} = -\beta \sum_p \langle p \,|\, \mathcal{H}_I \,|\, p \rangle e^{-\beta E_p} \,. \tag{3.7}$$

Clearly (3.3b) is the obvious (but nonunique) choice for $\mathscr{H}_I^{(1)}(D)$. This choice is convenient, as it automatically generates those terms in the perturbation series where *all* the sums over the states are restricted to the subspace P, such as the first term in (3.5c) and the first term in (3.5d). Consequently, the conditions on $\mathscr{H}_I^{(2)}(D)$ and $\mathscr{H}_I^{(3)}(D)$ are determined by the terms containing at least one set of intermediate states belonging to Q, and are exhibited in Appendix B. There it is also shown that the results (3.3b) for $\mathscr{H}_I^{(2)}(D)$ and (3.3d) for $\mathscr{H}_I^{(3)}(D)$ represent one possible choice satisfying these conditions. Again, there is no reason to expect any difficulties of principle in carrying out this procedure to higher orders in perturbation theory. The requirement that the recursion relations satisfy the semigroup property is an important one. The proof that choice (3.3) does meet this requirement is also part of Appendix B.

IV. THERMODYNAMIC SCALING THEORY APPLIED TO THE GENERALIZED IMPURITY HAMILTONIAN: RECURSION RELATIONS

In this section the formal scaling procedure developed in the preceding section is applied to the generalized impurity Hamiltonian with $\mathscr{U},\mathscr{V},\mathscr{S}$ being treated perturbatively. The essential result is that $\mathscr{H}_I(D)$ can also be written in the form (2.7) with $\mathscr{U}_D,\mathscr{V}_D,\mathscr{S}_D$ replacing $\mathscr{U},\mathscr{V},\mathscr{S}$; recursions relating the two are derived.

To proceed, divide the electron and hole creation operators $a^\dagger_{\epsilon\mu},b^\dagger_{\epsilon\mu}$ into the following two sets:

$$(a_{p\mu},b_{p\mu}) \text{ for } 0<p<D$$

and (4.1)

$$(a^\dagger_{q\mu},b^\dagger_{q\mu}) \text{ for } D<q<D_0\ .$$

Because of the definitions of the subspace P as containing *no* electrons or holes of energy $D<\epsilon<D_0$, one clearly has

$$a_{q\mu}P=b_{q\mu}P=Pa^\dagger_{q\mu}=Pb^\dagger_{q\mu}=0\ . \tag{4.2}$$

Hence one has the following results for operators such as $P\mathscr{H}_IP$, $Q\mathscr{H}_IQ$, $P\mathscr{H}_IQ$, etc. The expressions corresponding to $P\mathscr{H}_IP$ and $Q\mathscr{H}_IQ$ are essentially the same as in (2.7) *except that* for $P\mathscr{H}_IP$ the energy integrals in (2.7d) and (2.7e) are restricted to P, i.e., to $0<\epsilon<D$. Furthermore,

$$P\mathscr{H}_{I1}Q=0\ , \tag{4.3a}$$

$$P\mathscr{H}_{I2}Q=\int_{q,\mu}P[\mathscr{V}^\dagger(q,\mu)a_{q\mu}+b_{q\mu}\mathscr{V}(-q,\mu)]Q\ , \tag{4.3b}$$

$$\begin{aligned}P\mathscr{H}_{I3}Q=&\int_{p,\mu}\int_{q,\nu}P[a^\dagger_{p\mu}a_{q\nu}\mathscr{S}(p,\mu;q,\nu)+b_{p\mu}a_{q\nu}\mathscr{S}(-p,\mu;q,\nu)+b_{q\nu}a_{p\mu}\mathscr{S}(-q,\nu;p,\mu)-b^\dagger_{p\mu}b_{q\nu}\mathscr{S}(-p,\mu;-q,\nu)]Q\\&+\int_{q_1,\mu_1}\int_{q_2,\mu_2}P[b_{q_1\mu_1}a_{q_2\mu_2}\mathscr{S}(-q_1,\mu_1;q_2,\mu_2)]Q\ .\end{aligned} \tag{4.3c}$$

The operators $Q\mathscr{H}_IP$ are Hermitian conjugates of the above expressions.

One can now use the above results in the recursions (3.3) and carry out the sums over the intermediate states and obtain explicit expressions for $\mathscr{H}_I(D)$. Since the first-order result $P\mathscr{H}_IP$ *is* of the form (2.7) with the energy integrals in (2.7c) and (2.7d) being restricted to P, one has, for the first-order contributions to $\mathscr{U}_D,\mathscr{V}_D,\mathscr{S}_D$,

$$\mathscr{U}_D^{(1)}=\mathscr{U},\quad \mathscr{V}_D^{(1)}(\epsilon,\mu)=\mathscr{V}(\epsilon,\mu)\ ,\quad \mathscr{S}_D^{(1)}(\epsilon,\mu;\epsilon',\mu')=\mathscr{S}(\epsilon,\mu;\epsilon',\mu')\ . \tag{4.4}$$

The second-order result for $\mathscr{H}_I^{(2)}(D)$ can also be shown to be of the form of (2.7b)–(2.7e) with the conduction electrons being restricted to P and with the operators $\mathscr{U}_D,\mathscr{V}_D,\mathscr{S}_D$, replaced by their second-order contributions,

$$\begin{aligned}\mathscr{U}_D^{(2)}=&-\int_{q,\mu}[\mathscr{V}^\dagger(q,\mu)\mathscr{V}(q,\mu)+\mathscr{V}(-q,\mu)\mathscr{V}^\dagger(-q,\mu)]\frac{1-e^{-\beta q}}{q}\\&-\int_{p,\mu}\int_{q,\nu}[\mathscr{S}(-p,\mu;q,\nu)\mathscr{S}(q,\nu;-p,\mu)+\mathscr{S}(-q,\nu;p,\mu)\mathscr{S}(p,\mu;-q,\nu)]\frac{1-e^{-\beta(p+q)}}{(p+q)}\\&-\int_{q_1,\nu_1}\int_{q_2,\nu_2}\mathscr{S}(-q_1,\nu_1;q_2,\nu_2)\mathscr{S}(q_2,\nu_2;-q_1,\nu_1)\frac{1-e^{-\beta(q_1+q_2)}}{q_1+q_2}\ ,\end{aligned} \tag{4.5a}$$

$$\begin{aligned}\mathscr{V}_D^{(2)}(\epsilon,\mu)=-\tfrac{1}{2}\int_{q,\nu}\Bigg[&\mathscr{S}(\epsilon,\mu;q,\nu)\mathscr{V}(q,\nu)\left[\frac{1-e^{-\beta(q-\epsilon)}}{q-\epsilon}+\frac{1-e^{-\beta q}}{q}\right]\\&-\mathscr{V}^\dagger(-q,\nu)\mathscr{S}(\epsilon,\mu;-q,\nu)\left[\frac{1-e^{-\beta(q+\epsilon)}}{q+\epsilon}+\frac{1-e^{-\beta q}}{q}\right]\Bigg]\ ,\end{aligned} \tag{4.5b}$$

$$\begin{aligned}\mathscr{S}_D^{(2)}(\epsilon,\mu;\epsilon',\mu')=-\tfrac{1}{2}\int_{q,\nu}\Bigg[&\mathscr{S}(\epsilon,\mu;q,\nu)\mathscr{S}(q,\nu,\epsilon',\mu')\left[\frac{1-e^{-\beta(q-\epsilon)}}{q-\epsilon}+\frac{1-e^{-\beta(q-\epsilon')}}{q-\epsilon'}\right]\\&-\mathscr{S}(-q,\nu;\epsilon',\mu')\mathscr{S}(\epsilon,\mu;-q,\nu)\left[\frac{1-e^{-\beta(q+\epsilon')}}{q+\epsilon'}+\frac{1-e^{-\beta(q+\epsilon)}}{q+\epsilon}\right]\Bigg]\ ,\end{aligned} \tag{4.5c}$$

where it must be reemphasized that $\int_q$ stands for $\int_D^{D_0} dq\,\rho_0(\pm q)$ as appropriate.

The algebra that leads to the above results is perhaps tedious, but is sufficiently straightforward if one notes the following basic points: (i) For a given choice of terms drawn from $P\mathscr{H}_I Q$ and $Q\mathscr{H}_I P$ the energy denominators are fixed, and the sum over $|q\rangle\langle q|$ in (3.3c) can be replaced by the identity operator. (ii) The a_q's and b_q's in $P\mathscr{H}_I Q$ can be "matched" and "contracted" with the $a_q^\dagger$'s and $b_q^\dagger$'s in $Q\mathscr{H}_I P$, respectively; otherwise, they can be anticommuted and moved until a_q,b_q are next to (to the left of) P and $a_q^\dagger$'s and $b_q^\dagger$'s are next to (to the right of) P and this gives zero in view of (4.2). As an illustrative example, consider one of the terms arising from $\mathscr{H}_{I2}$ treated in second order given by

$$-\tfrac{1}{2}\int_{p,\mu}\int_{q,\nu}\int_{q',\nu'}\int_{p',\mu'} P[b_{q'\nu'}a_{p'\mu'}\mathscr{S}(-q',\nu';p',\mu')][\mathscr{S}(p,\mu;-q,\nu)a_{p\mu}^\dagger b_{q\nu}^\dagger]P \times\left[\frac{1-e^{-\beta(p+q)}}{p+q}+\frac{1-e^{-\beta(p'+q')}}{p'+q'}\right]. \tag{4.6}$$

Anticommuting the b_q's and $b_q^\dagger$'s, one has

$$P(b_{q'\nu'}a_{p'\mu'}a_{p\mu}^\dagger b_{q\mu}^\dagger)P=P[a_{p'\mu'}a_{p\mu}^\dagger(\delta_{qq'}\delta_{\nu\nu'}-b_{q\mu}^\dagger b_{q'\nu'})]P\ , \tag{4.7}$$

where the second term (with $b_{q'\nu'}P$) on the right-hand side can be dropped in view of (4.2). Normal ordering the remainder gives

$$\delta_{qq'}\delta_{\nu\nu'}(\delta_{pp'}\delta_{\mu\mu'}-Pa_{p\mu}^\dagger a_{p'\mu'})\ . \tag{4.8a}$$

It is easy to see that the first term above makes a contribution to $\mathscr{U}_D^{(2)}$ given by

TABLE I. Third-order contributions of the type $P\mathscr{H}_I Q\mathscr{H}_I Q\mathscr{H}_I P$ [i.e., arising from the first term in (3.3d)] to $\mathscr{S}_D(\epsilon,\mu;\epsilon',\mu')$ and $\mathscr{U}_D$ in the case when $\mathscr{V}=0$. Each of the operator terms listed is to be multiplied by the corresponding energy denominator term $h_1^{(3)}(E_a,E_b;E_{q_1},E_{q_2})$ [cf. (B11a)], which can be calculated using the energy differences listed and then integrated over repeated labels such as (q,ν), (p_1,μ_1), (q_1,μ_1), etc., with $\int_q=\int_D^{D_0}dq\,\rho_0(\pm q)$ and $\int_p=\int_0^D dp\,\rho_0(\pm p)$ as appropriate.

Operator		Energy differences	
	$E_{q_1}-E_a$	$E_{q_2}-E_b$	$E_{q_1}-E_{q_2}$
Contribution to $\mathscr{S}_D^{(3)}(\epsilon,\mu;\epsilon',\mu')$			
$\mathscr{S}(-p_1,\mu_1;q,\nu)\mathscr{S}(\epsilon,\mu;\epsilon',\mu')\mathscr{S}(q,\nu;-p_1,\mu_1)$	$q+p_1$	$q+p_1$	$\epsilon-\epsilon'$
$-\mathscr{S}(\epsilon,\mu;q,\nu)\mathscr{S}(-p_1,\mu_1;\epsilon',\mu')\mathscr{S}(q,\nu;-p_1,\mu_1)$	$q-\epsilon$	$q+p_1$	$-p_1-\epsilon'$
$-\mathscr{S}(-p_1,\mu_1;q,\nu)\mathscr{S}(\epsilon,\mu;-p_1,\mu_1)\mathscr{S}(q,\nu;\epsilon',\mu')$	$q+p_1$	$q-\epsilon'$	$\epsilon+p_1$
$\mathscr{S}(-q,\nu;p_1,\mu_1)\mathscr{S}(\epsilon,\mu;\epsilon',\mu')\mathscr{S}(p_1,\mu_1;-q,\nu)$	p_1+q	p_1+q	$\epsilon-\epsilon'$
$-\mathscr{S}(-q,\nu;p_1,\mu_1)\mathscr{S}(p_1,\mu_1;\epsilon',\mu')\mathscr{S}(\epsilon,\mu;-q,\nu)$	p_1+q	$\epsilon+q$	$p_1-\epsilon'$
$-\mathscr{S}(-q,\nu;\epsilon',\mu')\mathscr{S}(\epsilon,\mu;p_1,\mu_1)\mathscr{S}(p_1,\mu_1;-q,\nu)$	$\epsilon'+q$	p_1+q	$\epsilon-p_1$
$\mathscr{S}(-q,\mu_1;q_2,\mu_2)\mathscr{S}(\epsilon,\mu;\epsilon',\mu')\mathscr{S}(q_2,\mu_2;-q_1,\mu_1)$	q_2+q_1	q_2+q_1	$\epsilon-\epsilon'$
$-\mathscr{S}(-q_1,\mu_1;q_2,\mu_2)\mathscr{S}(q_2,\mu_2;\epsilon',\mu')\mathscr{S}(\epsilon,\mu;-q_1,\mu_1)$	q_2+q_1	$\epsilon+q_1$	$q_2-\epsilon'$
$-\mathscr{S}(-q_1,\mu_1;\epsilon',\mu')\mathscr{S}(\epsilon,\mu;q_2,\mu_2)\mathscr{S}(q_2,\mu_2;-q_1,\mu_1)$	$\epsilon'+q_1$	q_2+q_1	$\epsilon-q_2$
$-\mathscr{S}(\epsilon,\mu;q_1,\mu_1)\mathscr{S}(-q_2,\mu_2;\epsilon',\mu')\mathscr{S}(q_1,\mu_1;-q_2,\mu_2)$	$q_1-\epsilon$	q_1+q_2	$-q_2-\epsilon'$
$-\mathscr{S}(-q_1,\mu_1;q_2,\mu_2)\mathscr{S}(\epsilon,\mu;-q_1,\mu_1)\mathscr{S}(q_2,\mu_2;\epsilon',\mu')$	q_2+q_1	$q_2-\epsilon'$	$\epsilon+q_1$
$\mathscr{S}(\epsilon,\mu;q_1,\mu_1)\mathscr{S}(q_1,\mu_1;q_2,\mu_2)\mathscr{S}(q_2,\mu_2;\epsilon',\mu')$	$q_1-\epsilon$	$q_2-\epsilon'$	q_1-q_2
$\mathscr{S}(-q_1,\mu_1;\epsilon',\mu')\mathscr{S}(-q_2,\mu_2;-q_1,\mu_1)\mathscr{S}(\epsilon,\mu;-q_2,\mu_2)$	$\epsilon'+q_1$	$\epsilon+q_2$	$-q_2+q_1$
$\mathscr{S}(\epsilon,\mu;q,\nu)\mathscr{U}\mathscr{S}(q,\nu;\epsilon',\mu')$	$q-\epsilon$	$q-\epsilon'$	0
$-\mathscr{S}(-q,\nu;\epsilon',\mu')\mathscr{U}\mathscr{S}(\epsilon,\mu;-q,\nu)$	$\epsilon'+q$	$\epsilon+q$	0
$\mathscr{S}(-q,\nu;p_1,\mu_1)\mathscr{S}(p_1,\mu_1;p_2,\mu_2)\mathscr{S}(p_2,\mu_2;-q,\nu)$	p_1+q	p_2+q	p_1-p_2
$-\mathscr{S}(-p_1,\mu_1;q,\nu)\mathscr{S}(-p_2,\mu_2;-p_1,\mu_1)\mathscr{S}(q,\nu;-p_2,\mu_2)$	$q+p_1$	$q+p_2$	$-p_2+p_1$
$\mathscr{S}(-p,\mu;q_1,\nu_1)\mathscr{S}(q_1,\nu_1;q_2,\nu_2)\mathscr{S}(q_2,\nu_2;-p,\mu)$	q_1+p	q_2+p	q_1-q_2
$\mathscr{S}(-q_1,\nu_1;p,\mu)\mathscr{S}(p,\mu;q_2,\nu_2)\mathscr{S}(q_2,\nu_2;-q_1,\nu_1)$	$p+q_1$	q_2+q_1	$p-q_2$
$-\mathscr{S}(-q_1,\nu_1;p,\mu)\mathscr{S}(-q_2,\nu_2;-q_1,\nu_1)\mathscr{S}(p,\mu;-q_2,\nu_2)$	$p+q_1$	$p+q_2$	$-q_2+q_1$
$\mathscr{S}(-q_1,\nu_1;q_2,\nu_2)\mathscr{S}(q_2,\nu_2;p,\mu)\mathscr{S}(p,\nu;-q_1,\nu_1)$	q_2+q_1	$p+q_1$	q_2-p
$\mathscr{S}(-p,\mu;q,\nu)\mathscr{U}\mathscr{S}(q,\nu;-p,\mu)$	$q+p$	$q+p$	0
$\mathscr{S}(-q,\nu;p,\mu)\mathscr{U}\mathscr{S}(p,\mu;-q,\nu)$	$p+q$	$p+q$	0
$\mathscr{S}(-q_1,\mu_1;q_2,\mu_2)\mathscr{U}\mathscr{S}(q_2,\mu_2;-q_1,\mu_1)$	q_2+q_1	q_2+q_1	0

$$-\int_{p,\mu}\int_{q,\nu}\mathscr{S}(-q,\nu;p,\mu)\mathscr{S}(p,\mu;-q,\nu)\left[\frac{1-e^{-\beta(p+q)}}{p+q}\right], \tag{4.8b}$$

which is one of the terms in (4.5a). The second term in (4.8a) gives rise to the contribution to $\mathscr{S}_D^{(2)}$ corresponding to the second term of (4.5c). Similarly, the other terms of (4.5) can be obtained.

The third-order contribution $\mathscr{H}_I(D)$ can similarly be obtained with the use of the above procedure. For the purposes of this paper it is sufficient to present the results only for the case when $\mathscr{V}=0$. As these are too lengthy to be exhibited as equations we have listed them in Tables I and II. It must be noted that in addition to terms considered above the following additional terms arise:

$$\mathscr{H}_{I4}(D)=\int_{\epsilon,\mu}\int_{\epsilon',\mu'}[c^\dagger_{\epsilon\mu}c^\dagger_{\epsilon'\mu'}\mathscr{W}_{2,D}(\epsilon,\mu;\epsilon',\mu')+\text{H.c.}]\,, \tag{4.9a}$$

$$\mathscr{H}_{I5}(D)=\int_{\epsilon,\mu}\int_{\epsilon_1,\mu_1}\int_{\epsilon_2,\mu_2}[c^\dagger_{\epsilon\mu}c^\dagger_{\epsilon_1\mu_1}c_{\epsilon_2\mu_2}\mathscr{V}_{3,D}(\epsilon,\mu;\epsilon_1,\mu_1;\epsilon_2,\mu_2)+\text{H.c.}]\,, \tag{4.9b}$$

$$\mathscr{H}_{I6}(D)=\int_{\epsilon_1,\mu_1}\cdots\int_{\epsilon_4\mu_4}c^\dagger_{\epsilon_1\mu_1}c^\dagger_{\epsilon_2\mu_2}c_{\epsilon_3\mu_3}c_{\epsilon_4\mu_4}\mathscr{S}_{4,D}(\epsilon_1,\mu_1;\epsilon_2,\mu_2;\epsilon_3,\mu_3;\epsilon_4,\mu_4)\,. \tag{4.9c}$$

It will be shown in the next section that for impurity problems $\mathscr{V}_3$ and $\mathscr{S}_4$ constitute irrelevant variables in the RG sense and can hence be ignored (unless they are present, accompanied by large coefficients, in the initial Hamiltonian itself). $\mathscr{W}_2$ is a marginal variable, but (unless present initially) it is generated by the recursions only when $\mathscr{V}$ is present and the latter turns out to be a relevant variable. Thus, compared to $\mathscr{V}$ the effects of $\mathscr{W}_2$ are seldom worth considering. Hence, the most important aspect of the thermodynamics of the generalized impurity Hamiltonian can be discussed just in terms of $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$.

The scaling procedure that has been discussed so far gives rise to a continuous trajectory (as a function of decreasing cutoff D) of generalized impurity Hamiltonians, characterized by $\mathscr{U}_D$, $\mathscr{V}_D$, and $\mathscr{S}_D$, all of which describe the same low-temperature physics as the starting model Hamiltonian with cutoff D_0. Invoking the semigroup property of the scaling transformation discussed in the last section, one can obtain differential recursion relations for the variation of $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$ with D. For this purpose one has to start with the Hamiltonian with cutoff D, characterized by $\mathscr{U}_D$, etc., and scale D down to $D-\delta D$ to obtain $\mathscr{U}_{D-\delta D}$, etc. In Eqs. (4.5) one can hence replace $\int_q$ by $\delta D\rho_0(\pm D)$ as appropriate,

TABLE II. Third-order contributions of the type $P\mathscr{H}_IP\mathscr{H}_IQ\mathscr{H}_IP$ [i.e., arising from the second term in (3.3d)] to $\mathscr{S}_D(\epsilon,\mu;\epsilon',\mu')$ and $\mathscr{U}_D$ in the case when $\mathscr{V}=0$. Each of the operator terms listed is to be combined with its *Hermitian conjugate term* [in case of $\mathscr{S}_D$, this is obtained by taking the adjoint of the operator term *and* interchanging (ϵ,μ) with (ϵ',μ')]. Then it is to be multiplied by the corresponding energy denominator term $h_2^{(3)}(E_a,E_b;E_p,E_q)$ [cf. (B11b)], which can be calculated using the energy differences listed and then integrated over repeated labels such as (q,ν), (p_1,μ_1), (q_1,μ_1), etc., with $\int_q=\int_D^{D_0}dq\,\rho_0(\pm q)$ and $\int_p=\int_0^D dp\,\rho_0(\pm p)$ as appropriate.

Operator	Energy differences E_p-E_a	 E_q-E_b	 E_p-E_q
Contribution to $\mathscr{S}_D^{(3)}(\epsilon,\mu;\epsilon',\mu')$			
$\mathscr{S}(\epsilon,\mu;\epsilon',\mu')\mathscr{S}(-q,\nu;p_1,\mu_1)\mathscr{S}(p_1,\mu_1;-q,\nu)$	$\epsilon'-\epsilon$	p_1+q	$-q-p_1$
$\mathscr{S}(\epsilon,\mu;\epsilon',\mu')\mathscr{S}(-p_1,\mu_1;q,\nu)\mathscr{S}(q,\nu;-p_1,\mu_1)$	$\epsilon'-\epsilon$	$q+p_1$	$-p_1-q$
$\mathscr{S}(\epsilon,\mu;p_1,\mu_1)\mathscr{S}(p_1,\mu_1;q,\nu)\mathscr{S}(q,\nu;\epsilon',\mu')$	$p_1-\epsilon$	$q-\epsilon'$	p_1-q
$\mathscr{S}(-p_1,\mu_1;\epsilon',\mu')\mathscr{S}(-q,\nu;-p_1,\mu_1)\mathscr{S}(\epsilon,\mu;-q,\nu)$	$\epsilon'+p_1$	$\epsilon+q$	$-q+p_1$
$-\mathscr{S}(\epsilon,\mu;p_1,\mu_1)\mathscr{S}(-q,\nu;\epsilon',\mu')\mathscr{S}(p_1,\mu_1;-q,\nu)$	$p_1-\epsilon$	p_1+q	$-q-\epsilon'$
$-\mathscr{S}(-p_1,\mu_1;\epsilon',\mu')\mathscr{S}(\epsilon,\mu;q,\nu)\mathscr{S}(q,\nu;-p_1,\mu_1)$	$\epsilon'+p_1$	$q+p_1$	$\epsilon-q$
$\mathscr{S}(\epsilon,\mu;\epsilon',\mu')\mathscr{S}(-q_1,\nu_1;q_2,\nu_2)\mathscr{S}(q_2,\nu_2;-q_1,\nu_1)$	$\epsilon'-\epsilon$	q_2+q_1	$-q_1-q_2$
$\mathscr{U}\mathscr{S}(\epsilon,\mu;q,\nu)\mathscr{S}(q,\nu;\epsilon',\mu')$	0	$q-\epsilon'$	$\epsilon-q$
$-\mathscr{U}\mathscr{S}(-q,\nu;\epsilon',\mu')\mathscr{S}(\epsilon,\mu;-q,\nu)$	0	$\epsilon+q$	$-q-\epsilon'$
Contribution to $\mathscr{U}_0^{(3)}$			
$\mathscr{S}(-p_1,\mu_1;p_2,\mu_2)\mathscr{S}(p_2,\mu_2;q,\nu)\mathscr{S}(q,\nu;-p_1,\mu_1)$	p_2+p_1	$q+p_1$	p_2-q
$-\mathscr{S}(-p_1,\mu_1;p_2,\mu_2)\mathscr{S}(-q,\nu;-p_1,\mu_1)\mathscr{S}(p_2,\mu_2;-q,\nu)$	p_2+p_1	p_2+q	$-q+p_1$
$\mathscr{U}\mathscr{S}(-p,\mu;q,\nu)\mathscr{S}(q,\nu;-p,\mu)$	$q+p$	$q+p$	$-p-q$
$\mathscr{U}\mathscr{S}(-q,\nu;p,\mu)\mathscr{S}(p,\mu;-q,\nu)$	$p+q$	$p+q$	$-q-p$
$\mathscr{U}\mathscr{S}(-q_1,\mu_1;q_2,\mu_2)\mathscr{S}(q_2,\mu_2;-q_1,\mu_1)$	q_2+q_1	q_2+q_1	$-q_1-q_2$

and replace q by D. It is then easy to verify that to second order the differential recursion relations are

$$\frac{d\mathscr{U}_D}{dD}=\int_\mu[\mathscr{V}_D^\dagger(D,\mu)\mathscr{V}_D(D,\mu)\rho_0(D)+\mathscr{V}_D(-D,\mu)\mathscr{V}_D^\dagger(-D,\mu)\rho_0(-D)]\frac{1}{D}$$
$$+\int_{p,\mu}\int_\nu[\mathscr{S}_D(-p,\mu;D,\nu)\mathscr{S}_D(D,\nu;-p,\mu)\rho_0(D)+\mathscr{S}_D(-D,\mu;p,\mu)\mathscr{S}_D(p,\mu;-D,\nu)\rho_0(-D)]\frac{1}{D+p}\ , \tag{4.10a}$$

$$\frac{d\mathscr{V}_D(\epsilon,\mu)}{dD}=\tfrac{1}{2}\int_\nu\left[\mathscr{S}_D(\epsilon,\mu;D,\nu)\mathscr{V}_D(D,\nu)\rho_0(D)\left[\frac{1}{D}+\frac{1-e^{-\beta(D-\epsilon)}}{D-\epsilon}\right]\right.$$
$$\left.-\mathscr{V}_D^\dagger(-D,\nu)\mathscr{S}_D(\epsilon,\mu;-D,\nu)\rho_0(-D)\left[\frac{1}{D}+\frac{1}{D+\epsilon}\right]\right]\ , \tag{4.10b}$$

$$\frac{d\mathscr{S}_D(\epsilon,\mu;\epsilon',\mu')}{dD}=\tfrac{1}{2}\int_\nu\left[\mathscr{S}_D(\epsilon,\mu;D,\nu)\mathscr{S}_D(D,\nu;\epsilon',\mu')\rho_0(D)\left[\frac{1-e^{-\beta(D-\epsilon)}}{D-\epsilon}+\frac{1-e^{-\beta(D-\epsilon')}}{D-\epsilon'}\right]\right.$$
$$\left.-\mathscr{S}_D(-D,\nu;\epsilon',\mu')\mathscr{S}_D(\epsilon,\mu;-D,\nu)\rho_0(-D)\left[\frac{1}{D+\epsilon}+\frac{1}{D+\epsilon'}\right]\right]\ , \tag{4.10c}$$

where terms of order $e^{-\beta D}$ have been dropped unless necessary to ensure nonsingularity. Note that the term with the double integral over q in (4.5a) drops out of the differential recursion relations since it is of order $(\delta D)^2$. The third-order contributions to the right-hand sides of (4.10) can be written down straightforwardly from Tables I and II by similar manipulations. We will therefore not record them separately.

V. RENORMALIZATION GROUP ASPECTS

The scaling transformation discussed in the previous sections can be used to define a renormalization-group transformation (RGT) in the space of generalized impurity Hamiltonians. There is a technical difference between the scaling transformation and the RGT, as the latter is defined so as to be independent of the scale of the cutoff, while in (4.10) D appears explicitly.

The most convenient way to define the RGT is to redefine the conduction-electron degrees of freedom in terms of dimensionless energy variables, and to rescale the cutoff D after each stage of thinning the degrees of freedom so that the dimensionless cutoff at each stage of the recursion is unity. This is easily accomplished by defining, for each value of the cutoff D, new conduction-electron operators

$$\tilde{c}_{x\mu}\equiv[\rho_0(\epsilon)D]^{1/2}c_{\epsilon\mu},\quad \epsilon=xD,\quad -1<x<1\ , \tag{5.1}$$

and similarly for $\tilde{c}_{x\mu}^\dagger$, $\tilde{a}_{x\mu}$, etc. Clearly, from (2.2) one has

$$\{\tilde{c}_{x\mu},\tilde{c}_{x'\mu'}^\dagger\}=\delta_{\mu\mu'}\delta(x-x')\ . \tag{5.2}$$

It is easy to verify that, in terms of these conduction-electron variables, $\mathscr{H}_0(D)$, $\mathscr{H}_{I2}(D)$, and $\mathscr{H}_{I3}(D)$ become

$$\mathscr{H}_0(D)=D\int_{x,\mu}x\tilde{c}_{x\mu}^\dagger\tilde{c}_{x\mu}\ , \tag{5.3a}$$

$$\mathscr{H}_{I2}(D)=D\int_{x,\mu}\left[\frac{\rho_0(Dx)}{D}\right]^{1/2}\times[\mathscr{V}_D^\dagger(Dx,\mu)\tilde{c}_{x\mu}+\text{H.c.}]\ , \tag{5.3b}$$

$$\mathscr{H}_{I3}(D)=D\int_{x,\mu}\int_{x',\mu'}[\rho_0(Dx)\rho_0(Dx')]^{1/2}\tilde{c}_{x\mu}^\dagger\tilde{c}_{x'\mu'}\times\mathscr{S}_D(Dx,\mu;Dx',\mu')\ , \tag{5.3c}$$

where $\int_x$ now stands for $\int_{-1}^{1}dx$. Now define the following dimensionless quantities:

$$\tilde{\mathscr{H}}(D)\equiv\tilde{\mathscr{H}}_0(D)+\tilde{\mathscr{H}}_I(D)$$
$$\equiv[\mathscr{H}_0(D)+\mathscr{H}_I(D)]/D\ , \tag{5.4a}$$

$$\tilde{\mathscr{U}}_D\equiv\mathscr{U}/D\ , \tag{5.4b}$$

$$\tilde{\mathscr{V}}_D(x,\mu)\equiv[\rho_0(Dx)/D]^{1/2}\mathscr{V}_D(Dx,\mu)\ , \tag{5.4c}$$

$$\tilde{\mathscr{S}}_D(x,\mu;x',\mu')\equiv[\rho_0(Dx)\rho_0(Dx')]^{1/2}\times\mathscr{S}_D(Dx,\mu;Dx',\mu')\ . \tag{5.4d}$$

Then it is evident that $\tilde{\mathscr{H}}_D$ is a generalized impurity Hamiltonian with (dimensionless) cutoff 1, and can be expressed in terms of the dimensionless conduction-electron variables exactly in the form (2.3) or (when normal ordered) (2.7) with the dimensionless couplings $\tilde{\mathscr{U}}_D$, $\tilde{\mathscr{V}}_D$, and $\tilde{\mathscr{S}}_D$ replacing $\mathscr{U}$, $\mathscr{V}$, and $\mathscr{S}$. The above transformation also makes evident that the thermodynamics of the Hamiltonian determined by

$$\mathrm{Tr}\exp\left[-\frac{\mathscr{H}(D_0)}{k_BT}\right]=\mathrm{Tr}\exp\left[-\frac{\tilde{\mathscr{H}}(D_0)}{k_BT/D_0}\right]$$
$$\cong\mathrm{Tr}\exp\left[-\frac{\tilde{\mathscr{H}}(D)}{k_BT/D}\right] \tag{5.5}$$

depends only on the dimensionless variables (k_BT/D_0), $\tilde{\mathscr{U}}_{D_0}$, $\tilde{\mathscr{V}}_{D_0}$, and $\tilde{\mathscr{S}}_{D_0}$, or equivalently, via the scaling transformation, upon (k_BT/D), $\tilde{\mathscr{U}}_D$, $\tilde{\mathscr{V}}_D$, and $\tilde{\mathscr{S}}_D$.

The scaling transformation that was discussed earlier, and the rescaling in (5.4), defines a transformation connecting $\tilde{\mathscr{H}}_D$ to $\tilde{\mathscr{H}}_{D_0}$, and this is indeed a *renormalization-*

group transformation. In particular, the differential RGT that relates $\tilde{\mathscr{H}}_{D-\delta D}$ to $\tilde{\mathscr{H}}_D$ has the form

$$\frac{d\tilde{\mathscr{H}}_D}{d\ln(D_0/D)}=\mathscr{R}[\tilde{\mathscr{H}}_D]\,, \tag{5.6}$$

where the transformation $\mathscr{R}$ is now independent of D. This follows from the fact that the procedure for obtaining $\tilde{\mathscr{H}}_{D-\delta D}$ from $\tilde{\mathscr{H}}_D$ can be carried out entirely in terms of the dimensionless variables: Namely, by eliminating the dimensionless conduction electron and hole degrees of freedom between $(1-\delta D/D)$ and 1 and by rescaling the dimensionless cutoff back to 1, in exact analogy to what was done earlier. Either by such a procedure or by making use of (5.4) and the recursion relations (4.5) it is easy to derive the recursion relations for $\tilde{\mathscr{U}}_D$, $\tilde{\mathscr{V}}_D$, and $\tilde{\mathscr{S}}_D$ explicitly. Up to second order these recursions read as follows [compare (4.5) and (4.10)]:

$$\frac{d\tilde{\mathscr{U}}_D}{d\ln(D_0/D)}=\tilde{\mathscr{U}}_D-\int_\mu[\tilde{\mathscr{V}}_D^\dagger(1,\mu)\tilde{\mathscr{V}}_D(1,\mu)+\tilde{\mathscr{V}}_D(-1,\mu)\tilde{\mathscr{V}}_D^\dagger(-1,\mu)]$$
$$-\int_{x,\mu}\int_\nu\frac{1}{1+x}[\tilde{\mathscr{S}}_D(-x,\mu;1,\nu)\tilde{\mathscr{S}}_D(1,\nu;-x,\mu)+\tilde{\mathscr{S}}_D(-1,\nu;x,\mu)\tilde{\mathscr{S}}_D(x,\mu;-1,\nu)] \tag{5.7a}$$

$$\frac{d\tilde{\mathscr{V}}_D(x,\mu)}{d\ln(D_0/D)}=\frac{\tilde{\mathscr{V}}_D}{2}-x\frac{\partial}{\partial x}\tilde{\mathscr{V}}_D(x,\mu)-\tfrac{1}{2}\int_\nu\left[\tilde{\mathscr{S}}_D(x,\mu;1,\nu)\tilde{\mathscr{V}}_D(1,\nu)\left[\frac{1-e^{\tilde{\beta}_D(1-x)}}{1-x}+1\right]\right.$$
$$\left.-\tilde{\mathscr{V}}_D^\dagger(-1,\nu)\tilde{\mathscr{S}}_D(x,\mu;-1,\nu)\left[1+\frac{1}{1+x}\right]\right], \tag{5.7b}$$

$$\frac{d\tilde{\mathscr{S}}_D(x,\mu;x',\mu')}{d\ln(D_0/D)}=-\left[x\frac{\partial}{\partial x}+x'\frac{\partial}{\partial x'}\right]\tilde{\mathscr{S}}_D(x,\mu;x',\mu')$$
$$-\tfrac{1}{2}\int_\nu\left[\tilde{\mathscr{S}}_D(x,\mu;1,\nu)\tilde{\mathscr{S}}_D(1,\nu;x',\mu')\left[\frac{1-e^{-\tilde{\beta}_D(1-x)}}{1-x}+\frac{1-e^{-\tilde{\beta}_D(1-x')}}{1-x'}\right]\right.$$
$$\left.-\tilde{\mathscr{S}}_D(-1,\nu;x',\mu')\tilde{\mathscr{S}}_D(x,\mu;-1,\nu)\left[\frac{1}{1+x}+\frac{1}{1+x'}\right]\right], \tag{5.7c}$$

where $\tilde{\beta}_D$ stands for the inverse scaled temperature:[23]

$$\tilde{\beta}_D=\beta D=(\beta D_0)(D/D_0)\,. \tag{5.8}$$

One important difference between these RGT recursions and the scaling equations (4.10) is the presence of the first-order terms on the right-hand side; these have arisen entirely out of the rescaling transformation (5.4). It must be emphasized that the above RG recursion relations (5.7) give only a specific perturbative realization of $\mathscr{R}$, but $\mathscr{R}$ itself (in the sense of the scheme of eliminating the high-energy conduction electrons and holes and rescaling) has meaning in an abstract, nonperturbative sense. For example, the numerical RG method developed by Wilson[24] is essentially a nonperturbative realization of $\mathscr{R}$ and is hence much more powerful. Yet another realization could be obtained by carrying out the elimination of the conduction-electron degrees of freedom by treating $\tilde{\mathscr{U}}_D$ not as a perturbation, but exactly as part of $\mathscr{H}_0$.

In fact, the particular realization of $\mathscr{R}$ embodied in Eqs. (5.7) constitute nothing but the perturbative RG recursions relations around what might be called the "free-impurity fixed point" of $\mathscr{R}$. The reason is that if $\tilde{\mathscr{U}}_D$, $\tilde{\mathscr{V}}_D$, and $\tilde{\mathscr{S}}_D$ were zero, $\tilde{\mathscr{H}}_0$ would just be $\tilde{\mathscr{H}}_0(D)$, which is characterized by a one-electron density of states $\rho_0(Dx)$ and if, furthermore, $\rho_0(\epsilon)$ is a constant ρ_0, then $\tilde{\mathscr{H}}_0(D)$ is independent of D and is a fixed point of $\mathscr{R}$. Physically, this free impurity fixed point corresponds to the situation in which all the states of the impurity are degenerate, and are decoupled from the conduction electrons. Now $\tilde{\mathscr{U}}_D$, $\tilde{\mathscr{V}}_D$, and $\tilde{\mathscr{S}}_D$ constitute deviations of $\tilde{\mathscr{H}}_D$ from this fixed point, and indeed the recursion relations (5.7) are the nonlinear RG equations for these deviations, and are valid only when these dimensionless couplings are small (compared to unity).

Examination of the linear terms in the RG recursions (5.7) shows that $\tilde{\mathscr{U}}_D$ and the energy-independent part of $\tilde{\mathscr{V}}_D$ constitute relevant deviations, the energy-independent parts of $\tilde{\mathscr{S}}_D$ constitute marginal deviations, and the energy-dependent parts of $\tilde{\mathscr{V}}_D$ and $\tilde{\mathscr{S}}_D$ constitute irrelevant deviations around the free-impurity fixed point. This can be seen by Taylor expanding $\tilde{\mathscr{V}}_D(x,\mu)$ and $\tilde{\mathscr{S}}_D(x,\mu;x',\mu')$ in powers of x and x', which is justified as $\tilde{\mathscr{V}}_D$ and $\tilde{\mathscr{S}}_D$ must both be *smooth* functions of the energy variables in order that they describe the interaction of conduction electrons with localized impurity states. Then one has

$$\tilde{\mathscr{V}}_D(x,\mu)=\sum_n\tilde{\mathscr{V}}_{D;n}(\mu)\frac{x^n}{n!}\,, \tag{5.9a}$$

$$\tilde{\mathscr{S}}_D(x,\mu;x',\mu')=\sum_{n,n'}\tilde{\mathscr{S}}_{D;n,n'}(\mu,\mu')\frac{x^n}{n!}\frac{(x')^{n'}}{(n')!}\,. \tag{5.9b}$$

Clearly, from the linear terms in (5.7b) and (5.7c) $\tilde{\mathscr{V}}_{D;n}$ has eigenvalue $(\frac{1}{2}-n)$ and $\tilde{\mathscr{S}}_{d;n,n'}$ has eigenvalue $-(n+n')$. In the same way, one can also verify that the dimensionless couplings $\tilde{\mathscr{V}}_{3,D}$ and $\tilde{\mathscr{S}}_{4,D}$ obtained by rescaling $\mathcal{H}_{15}(D)$ and $\mathcal{H}_{16}(D)$ defined in Eq. (4.9) constitute irrelevant deviations, and that the energy-independent part of $\tilde{\mathcal{W}}_{2,D}$ constitutes a marginal deviation.

Next we discuss the question of how the scaling procedure relates to the calculation of the thermodynamic properties of $\mathcal{H}$ at a temperature T (typically $k_B T \ll D_0$). The basic strategy is that one carries out the scaling until D is reduced to $10T$ during the entirety of which the approximation of neglecting terms of order $\exp(-D/T)$ is justified. Suppose that during this entire process $\tilde{\mathcal{U}}_D$, $\tilde{\mathcal{V}}_D$, and $\tilde{\mathcal{S}}_D$ continue to remain small so that the higher-order terms which should in principle be present in the recursions (5.7) can be neglected. Then one can integrate these recursion relations until $D=10T$, and thereby obtain the final scaled Hamiltonian, to be denoted $\tilde{\mathcal{H}}_{\text{eff}}(T)$, and calculate the thermodynamics from $\operatorname{Tr}\exp[-10\tilde{\mathcal{H}}_{\text{eff}}(T)]$ [cf. Eq. (5.5)]. The point is such that a calculation can be done perturbatively in terms of $\tilde{\mathcal{U}}_{\text{eff}}(T)$, $\tilde{\mathcal{V}}_{\text{eff}}(T)$, and $\tilde{\mathcal{S}}_{\text{eff}}(T)$, and will result in *good expansions,* i.e., expansions free of divergences, since the effective ratio of the cutoff to the temperature in $\tilde{\mathcal{H}}_{\text{eff}}(T)$ is fixed to be 10 by definition. In fact, such a procedure can be shown to be equivalent to summing up specific infinite subsets of terms in perturbation theory. This will be illustrated in the next section with the use of a specific example.

Of course, in general, $\tilde{\mathcal{U}}_D$, $\tilde{\mathcal{V}}_D$, and $\tilde{\mathcal{S}}_D$ do not remain small once D/D_0 becomes sufficiently small, since $\tilde{\mathcal{U}}_D$ and $\tilde{\mathcal{V}}_{D;0}$ are relevant and $\tilde{\mathcal{S}}_{D;0,0}$ can be marginally unstable. In this case perturbative RG equations such as (5.7) break down when any of the dimensionless couplings become of order unity. *However, this does not render perturbative scaling useless* because $\mathcal{R}$ has a nonperturbative meaning, and so do $\tilde{\mathcal{H}}_D$ and $\tilde{\mathcal{H}}_{\text{eff}}(T)$. Indeed, the numerical RG methods developed by Wilson permit one to follow the trajectory of $\tilde{\mathcal{H}}_{\text{eff}}(T)$ with decreasing T even when any of the effective couplings become large. The understanding of the general character of the trajectory of $\tilde{\mathcal{H}}_{\text{eff}}(T)$ gained by the application of these methods to many problems suggests the following method of *using perturbative scaling repeatedly to trace pieces of the trajectory of* $\tilde{\mathcal{H}}_{\text{eff}}(T)$.

The method depends on the fact that typically,[14] the trajectories of $\tilde{\mathcal{H}}_{\text{eff}}(T)$, or equivalently of $\tilde{\mathcal{H}}(D)$, are in the form of flows from the neighborhood of one fixed point of $\mathcal{R}$ to that of another, and that the crossover of $\tilde{\mathcal{H}}(D)$ away from a fixed point takes place when one of the relevant or marginally unstable deviations around the fixed point becomes of order unity. What is more significant is that the fixed points *often* correspond to some new effective impurity degree of freedom with all its states degenerate and decoupled from the conduction electrons. Hence, when D (or T) is in the regime of such a fixed point, i.e., such that $\tilde{\mathcal{H}}(D)$ [or $\tilde{\mathcal{H}}_{\text{eff}}(T)$] is in the neighborhood of this fixed point, $\tilde{\mathcal{H}}(D)$ can once again be represented as a new generalized impurity Hamiltonian with new dimensionless couplings. Furthermore, new RG recursion relations can be written down with the use of (5.7); solving these relations permits one to trace the trajectory of $\tilde{\mathcal{H}}(D)$ as long as it stays in the vicinity of that fixed point. In other words, the entire range of T (or D) can be broken up into various regimes in each of which $\tilde{\mathcal{H}}_{\text{eff}}(T)$ is in the neighborhood of some fixed point of the RG transformation $\mathcal{R}$. Also in each of these regimes, the physics of the problem can often be understood in simple perturbative terms, albeit these terms are of undetermined "phenomenological" parameters that specify the various dimensionless couplings in each regime. Of course, to connect such phenomenological parameters to the coupling constants of the initial model Hamiltonian one must be able to follow the trajectory of $\tilde{\mathcal{H}}(D)$ through its crossover regimes. While this can be done with the use of the perturbative scaling equations occasionally, in general it requires the use of nonperturbative realizations of $\mathcal{R}$. For a textbook illustration of the various ideas presented above, their power and their limitations, the interested reader is directed to our treatment of the two-impurity Kondo problem.[13]

VI. ILLUSTRATION OF THE USE OF THE THERMODYNAMIC SCALING TECHNIQUES: THE SINGLE-IMPURITY KONDO PROBLEM

In this section we apply the methods discussed so far to the single-impurity (isotropic) Kondo problem. This is a well-studied and reasonably well-understood problem, so our purpose is partly to check that our methods reproduce known results and partly to bring out some of the subtle aspects associated with the use of these scaling methods.

As discussed in Sec. II, in case of the single-impurity Kondo problem μ stands for the spin label only, and in the model Hamiltonian one has

$$\mathcal{U}=\mathcal{V}=0,\quad \mathcal{S}(\epsilon,\alpha;\epsilon',\alpha')=-\frac{J_0}{2}\vec{S}\cdot\vec{\sigma}_{\alpha\alpha'}\,, \tag{6.1}$$

where $\vec{S}$ represents the impurity spin. For concreteness, it will be assumed hereafter that the density of states $\rho_0(\epsilon)$ is a constant, ρ_0. It is then just a question of straightforward, albeit tedious, spin algebra to work out $\mathcal{U}_D$ and $\mathcal{S}_D$ ($\mathcal{V}_D=0$ for all D) using the relations (4.5) and Tables I and II.

Consider the second-order results. One has

$$\mathcal{U}_D^{(2)}=-\frac{(\rho_0 J_0)^2}{4}\left[\int_0^D dp\int_D^{D_0} dq\, S^i S^j[\operatorname{Tr}(\sigma^i\sigma^j)+\operatorname{Tr}(\sigma^j\sigma^i)]\frac{1-e^{-\beta(p+q)}}{p+q}\right.$$
$$\left.+\int_D^{D_0} dq_1\int_D^{D_0} dq_2\, S^i S^j[\operatorname{Tr}(\sigma^i\sigma^j)]\frac{1-e^{-\beta(q_1+q_2)}}{q_1+q_2}\right], \tag{6.2a}$$

$$\mathscr{S}_D^{(2)}(\epsilon,\alpha;\epsilon',\alpha')=-\tfrac{1}{8}\rho_0 J_0^2 \int_D^{D_0} dq\, S^i S^j \left[(\sigma^i\sigma^j)_{\alpha\alpha'}\left[\frac{1-e^{-\beta(q-\epsilon)}}{q-\epsilon}+\frac{1-e^{-\beta(q-\epsilon')}}{q-\epsilon'}\right] - (\sigma^j\sigma^i)_{\alpha\alpha'}\left[\frac{1-e^{-\beta(q+\epsilon')}}{q+\epsilon'}+\frac{1-e^{-\beta(q+\epsilon)}}{q+\epsilon}\right]\right] . \tag{6.2b}$$

Using

$$\sigma^i\sigma^j=\delta_{ij}+i\epsilon^{ijk}\sigma^k \text{ and } \epsilon^{ijk}S^iS^j=iS^k , \tag{6.3}$$

performing the integrals, and dropping terms of order $e^{-\beta D}$ and $e^{-\beta(D_0-D)}$, one obtains

$$\mathscr{U}_D^{(2)}=-(\rho_0 J_0)^2 S(S+1)(D_0-D)\ln 2\equiv E_D^{(2)} , \tag{6.4}$$

$$\mathscr{S}_D^{(2)}(\epsilon,\alpha;\epsilon',\alpha')\equiv K_D^{(2)}(\epsilon,\epsilon')\delta_{\alpha\alpha'}-\tfrac{1}{2}J_D^{(2)}(\epsilon,\epsilon')\vec{\mathrm{S}}\cdot\vec{\sigma}_{\alpha\alpha'} , \tag{6.5a}$$

where

$$K_D^{(2)}(\epsilon,\epsilon')=-\frac{\rho_0 J_0^2}{8}S(S+1)\left[\mathrm{Ei}(-\beta(D-\epsilon))+\ln\left|\frac{D_0-\epsilon}{D-\epsilon}\,\frac{D+\epsilon}{D_0+\epsilon}\right|+(\epsilon\to\epsilon')\right] , \tag{6.5b}$$

$$J_D^{(2)}(\epsilon,\epsilon')=-\frac{\rho_0 J_0^2}{4}S(S+1)\left[\mathrm{Ei}(-\beta(D-\epsilon))+\ln\left|\frac{D_0-\epsilon}{D-\epsilon}\,\frac{D_0+\epsilon}{D+\epsilon}\right|+(\epsilon\to\epsilon')\right] . \tag{6.5c}$$

Note that the only temperature dependence of the couplings is generated via the exponential integral function $\mathrm{Ei}(x)$ and is hence negligible unless $|D-\epsilon|$ or $|D-\epsilon'|<k_B T$. Note that the form of the results (6.4) and (6.5) is consistent with the symmetries, namely rotational invariance and particle-hole symmetry, present in the problem. In particular, $\mathscr{U}_D$ can only be a trivial constant and $K(\epsilon,\epsilon')$ has no energy-independent component, i.e., there is no contact potential scattering.

One can similarly work out the algebra for the third-order results and verify that $\mathscr{U}_D^{(3)}$ is also a constant $E_D^{(3)}$, and that $\mathscr{S}_D^{(3)}$ is also of the form (6.5a). For the purposes of this paper, it is enough to exhibit the result for the energy-independent part of $J_D(\epsilon,\epsilon')$, i.e., $J_D(0,0)$, to be denoted $J(D)$. One has

$$J^{(3)}(D)=\tfrac{1}{2}\rho_0^2 J_0^3\left[\ln^2\left[\frac{D_0}{D}\right][S(S+1)+1]-\ln\left[\frac{D_0}{D}\right]-(2I_1-I_2)[S(S+1)-1]+I_3[S(S+1)+1]\right] , \tag{6.6}$$

where

$$I_1\equiv\int_D^{D_0}\frac{dq}{q}\ln\left|\frac{D_0+q}{q}\right| , \tag{6.7a}$$

$$I_2\equiv\int_D^{D_0}\frac{dq}{q}\ln\left|\frac{D+q}{q}\right| , \tag{6.7b}$$

$$I_3\equiv\int_D^{D_0}\frac{dq}{q}I_4(q)\equiv\int_D^{D_0}\frac{dq}{q}\int_0^D d\epsilon\left[\frac{e^{-\beta(q-\epsilon)}-1}{q-\epsilon}+e^{-\beta q}\left[\frac{e^{\beta\epsilon}-1}{\epsilon}\right]\right] . \tag{6.7c}$$

Note that the result (6.6) has contributions coming from both the sets (Tables I and II) of third-order terms. It is quite clear that $J_D^{(2)}$ and $J_D^{(3)}$ have logarithmic terms involving $\ln(D_0/D)$, and since the thermodynamic properties of $\mathscr{H}$ at temperature T are supposed to have good expansions in powers of J_D for D of the order of T, their expansions in powers of J_0 will have logarithmic terms involving $\ln(D_0/T)$ as stated in Sec. III.

Next consider the recursion relations. The dimensionless couplings are given by [cf. (5.4)]

$$\tilde{\mathscr{U}}_D=\tilde{E}_D\equiv\frac{E_D}{D} , \tag{6.8a}$$

$$\tilde{\mathscr{S}}_D(x,\alpha;x',\alpha')=\rho_0\mathscr{S}_D(Dx,\alpha;Dx',\alpha') , \tag{6.8b}$$

and in view of (6.5a) one expects that

$$\tilde{\mathscr{S}}_D(x,\alpha;x',\alpha')=\tilde{K}_D(x,x')-\tfrac{1}{2}\tilde{J}_D(x,x')\vec{\mathrm{S}}\cdot\vec{\sigma}_{\alpha\alpha'} , \tag{6.9a}$$

where

$$\tilde{K}_D(x,x')=\rho_0 K_D(Dx,Dx'),\quad \tilde{J}_D(x,x')=\rho_0 J_D(Dx,Dx') . \tag{6.9b}$$

Substituting these forms into (5.7) and going through the same algebra as before now enables one to write down recursion relations for $\tilde{E}_D$, $\tilde{K}_D$, and $\tilde{J}_D$. They are given by

$$\frac{d\tilde{E}_D}{d\ln(D_0/D)}=\tilde{E}_D-\int_0^1\frac{dx}{1+x}\left\{2[\tilde{K}_D(-x,1)\tilde{K}_D(1,-x)+\tilde{K}_D(-1,x)\tilde{K}_D(x,-1)]\right.$$
$$\left.+\frac{S(S+1)}{2}[\tilde{J}_D(-x,1)\tilde{J}_D(1,-x)+\tilde{J}_D(-1,x)\tilde{J}_D(x,-1)]\right\},\tag{6.10a}$$

$$\frac{d\tilde{K}_D(x,x')}{d\ln(D_0/D)}=-\left\{x\frac{\partial}{\partial x}+x'\frac{\partial}{\partial x'}\right\}\tilde{K}_D(x,x')$$
$$-\tfrac{1}{2}\left[\left\{\tilde{K}_D(x,1)\tilde{K}_D(1,x')+\frac{S(S+1)}{4}\tilde{J}_D(x,1)\tilde{J}_D(1,x')\right\}\left\{\frac{1-e^{-\beta_D(1-x)}}{1-x}+(x\to x')\right\}\right.$$
$$\left.-\left\{\tilde{K}_D(x,-1)\tilde{K}_D(-1,x')+\frac{S(S+1)}{4}\tilde{J}_D(x,-1)\tilde{J}_D(-1,x')\right\}\left\{\frac{1}{1+x}+\frac{1}{1+x'}\right\}\right],\tag{6.10b}$$

$$\frac{d\tilde{J}_D(x,x')}{d\ln(D_0/D)}=-\left\{x\frac{\partial}{\partial x}+x'\frac{\partial}{\partial x'}\right\}\tilde{J}_D(x,x')$$
$$-\tfrac{1}{4}\left[[\tilde{J}_D(x,1)\tilde{J}_D(1,x')+2\tilde{K}_D(x,1)\tilde{J}_D(1,x')+2\tilde{J}_D(x,1)\tilde{K}_D(1,x')]\left\{\frac{1-e^{-\beta_D(1-x)}}{1-x}+(x\to x')\right\}\right.$$
$$\left.+[\tilde{J}_D(x,-1)\tilde{J}_D(-1,x')-2\tilde{K}_D(x,-1)\tilde{J}_D(-1,x')-2\tilde{J}_D(x,-1)\tilde{K}_D(-1,x')]\left\{\frac{1}{1+x}+\frac{1}{1+x'}\right\}\right].\tag{6.10c}$$

It must be emphasized that if one keeps track of the energy dependence of $\tilde{J}_D(x,x')$ and $\tilde{K}_D(x,x')$, these are recursion relations for infinitely many variables, even though all of them except for $\tilde{J}_D(0,0)$, to be denoted $\tilde{J}(D)$, constitute irrelevant variables *about the local moment* (LM) *fixed point* (which corresponds to $\mathcal{J}_D=0$, i.e., to the impurity spin being decoupled from the conduction electrons). This is seen, as before, by expanding $\tilde{J}_D(x,x')$ and $\tilde{K}_D(x,x')$ in a Taylor series as in (5.9). One thus has

$$\tilde{J}_D(x,x')=\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\tilde{J}_{D;n_1,n_2}\frac{(x)^{n_1}}{n_1!}\frac{(x')^{n_2}}{n_2!},\tag{6.11a}$$

$$\tilde{K}_D(x,x')=\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\tilde{K}_{D;n_1,n_2}\frac{(x)^{n_1}}{n_1!}\frac{(x')^{n_2}}{n_2!}.\tag{6.11b}$$

Converting the recursions (6.10) into recursions for $\tilde{J}_{D;n_1,n_2}$ and $\tilde{K}_{D;n_1,n_2}$ one notes from the linear part of the recursion relations that both $\tilde{J}_{D;n_1,n_2}$ and $\tilde{K}_{D;n_1,n_2}$ have eigenvalues $-(n_1+n_2)$. But $\tilde{K}_{D;0,0}$ is not generated by the recursion relation and hence $\tilde{J}_{D;0,0}$, which is the same as $J(D)$, is the only marginal variable and is the dominant coupling constant in the problem, and all other variables are irrelevant variables.

As a first approximation, therefore, one might think that it is sufficient to consider the recursion relations for $\tilde{J}(D)$ alone and ignore all other coupling constants. It is easy to derive these up to third order, indeed just by inspection of Eqs. (6.5e) and (6.6). The results are the following:

$$\frac{d\tilde{J}}{d\ln(D_0/D)}=-\tilde{J}^2-\frac{\tilde{J}^3}{2}\{1+[S(S+1)-1]\ln2$$
$$-[S(S+1)+1]I_4\},\tag{6.12}$$

where I_4 is just the inner integral, over ϵ, in (6.7c) evaluated at $q=D$ (cf. Appendix C) and is given by [cf. Eq. (C7b)]

$$I_4=e^{-\beta D}[\mathrm{Ei}(\beta D)-\ln(\beta D)-\gamma]$$
$$+[\mathrm{Ei}(-\beta D)-\ln(\beta D)-\gamma],\tag{6.13}$$

where γ is Euler's constant. This does not agree with result (1.2) and is indeed wrong because the approximation ignoring all couplings other than $\tilde{J}$, even if they be irrelevant, is invalid.

In order to see this let $\tilde{G}_i$ label all the irrelevant variables and λ_i their eigenvalues. Then the recursion relations will clearly be of the form

$$\frac{d\tilde{J}}{dt}=a_2\tilde{J}^2+a_3\tilde{J}^3+\sum_i b_i\tilde{J}\tilde{G}_i+\cdots,\tag{6.14a}$$

$$\frac{d\tilde{G}_i}{dt}=-\lambda_i+c_i\tilde{J}^2+\cdots,\tag{6.14b}$$

where the ellipses stand for other terms unimportant for the ensuing discussion and where for convenience D has been parametrized as

$$D=D_0e^{-t}\ ,$$

i.e., (6.14c)

$$\ln(D_0/D)=t\ .$$

Indeed, the two terms in (6.12) correspond to the first two terms of (6.14a). Now one must note that, although $\tilde{G}_i$ decreases because of the negative eigenvalues of λ_i as t increases, they are constantly generated to order $\tilde{J}^2$ via the second term in (6.14b). Thus the $\tilde{G}_i$ affect $d\tilde{J}/dt$ to order $\tilde{J}^3$ via the third term of (6.14a). Hence, $d\tilde{J}/dt$ cannot be obtained to third order correctly if all the irrelevant variables are neglected outright. The way to treat this problem is to solve the equations iteratively as suggested by Wilson[25]: Integrating (6.14b), one has [since $\tilde{G}_i(t=0)=0$]

$$\tilde{G}_i(t)=c_i\int_0^t e^{-\lambda_i(t-t')}dt'[\tilde{J}(t')]^2 \tag{6.15a}$$

$$\cong c_i[\tilde{J}(t)]^2\left[\frac{1-e^{-\lambda_i t}}{\lambda_i}\right]+O(\tilde{J}^3) \tag{6.15b}$$

$$\cong c_i\frac{[\tilde{J}(t)]^2}{\lambda_i}\ , \tag{6.15c}$$

(6.15b) is obtained by noting that (6.15a) is dominated by t of the order of t' and by Taylor expanding $\tilde{J}(t')$ around $\tilde{J}(t)$ and using (6.14a); Eq. (6.15c) is justified because $e^{-\lambda_i t}=(D/D_0)^{\lambda_i}$ can be neglected for $D \ll D_0$. Hence one gets

$$\frac{d\tilde{J}}{dt}=a_2\tilde{J}^2+\left[a_3+\sum_i\frac{b_ic_i}{\lambda_i}\right]\tilde{J}^3\ . \tag{6.16}$$

Thus, to obtain the correct third-order scaling equations for $\tilde{J}$ alone, the scaling procedure one adopts must correctly handle the coupling of $\tilde{J}$ to all the irrelevant variables in second order. We demonstrate below that our scaling procedure does this, not by directly using (6.16) but by a simpler alternative procedure.

The demonstration is based on the idea of "good expansions" discussed by Wilson,[25] where he has shown on general grounds that for a problem with a single marginal variable, as is seen here, $(d\tilde{J}/dt)$ must have a good expansion in terms of $\tilde{J}$ and one can obtain such an expansion by inverting the perturbation series for $\tilde{J}$ $[\equiv\rho_0 J(D)]$ in terms of $\tilde{J}_0$ $[\equiv\rho_0 J_0]$ as follows: With the use of (6.5c) and (6.6) one can obtain an expansion for $\tilde{J}$ in powers of $\tilde{J}_0$ in the form

$$\tilde{J}(t)=\tilde{J}_0+A_2(t)\tilde{J}_0^2+A_3(t)\tilde{J}_0^3+\cdots\ ,$$

where, neglecting terms of order $(e^{-\beta D})$, one has

$$A_2(t)=-\ln(D_0/D)=-t\ , \tag{6.17a}$$

$$\begin{aligned}A_3(t)=\tfrac{1}{2}\{&t^2[S(S+1)+1]-t\\&-[2I_1(t)-I_2(t)][S(S+1)-1]\\&+I_3(t)[S(S+1)+1]\}\ .\end{aligned} \tag{6.17b}$$

Here $I_1(t)$, $I_2(t)$, and $I_3(t)$ are obtained by setting $D=D_0e^{-t}$ in (6.7). Equation (6.17) is a *bad expansion* for large t (small D/D_0) since $A_2(t)$ and $A_3(t)$ can become large. From it two more bad expansions can be obtained; one by differentiating (6.17a) to get $d\tilde{J}/dt$ in terms of $\tilde{J}_0$ and another by inverting (6.17a) to get $\tilde{J}_0$ in terms of $\tilde{J}$:

$$\frac{d\tilde{J}}{dt}=A_2'(t)\tilde{J}_0^2+A_3'(t)\tilde{J}_0^3+\cdots\ , \tag{6.18}$$

$$\tilde{J}_0=\tilde{J}-A_2(t)\tilde{J}^2+\{2[A_2(t)]^2-A_3(t)\}\tilde{J}^3+\cdots\ .$$

However, the important point is that the expansion obtained by substituting (6.19) in (6.18), namely

$$\frac{d\tilde{J}}{dt}=A_2'(t)\tilde{J}^2+[A_3'(t)-2A_2(t)A_2']\tilde{J}^3+\cdots\ , \tag{6.20}$$

is expected to be a good expansion, and to be the same as (6.16) [provided that irrelevant variables have been correctly handled in obtaining the expansion (6.17a)]. From (6.17b), $A_2'=-1$, and it is shown in Appendix C that

$$[A_3'(t)-2A_2(t)A_2']=-\tfrac{1}{2}$$

if one neglects terms of order (D/D_0) and (T/D). Hence one has

$$\frac{d\tilde{J}}{dt}=\alpha_2\tilde{J}^2+\alpha_3\tilde{J}^3+\cdots=-\tilde{J}^2-\tfrac{1}{2}\tilde{J}^3+\cdots\ , \tag{6.21}$$

in agreement with earlier results. Note that our formalism permits the evaluation of the order (T/D) corrections to α_3, the coefficient of the $\tilde{J}^3$ term in (6.21); these corrections may be significant for quantitative calculations. But they will be ignored for the purposes of the ensuing discussions.

There are several important aspects connected with recursion relations such as (6.21) that are worth reemphasizing, even if they have been discussed elsewhere in the literature.[26] First, one can integrate (6.21) to obtain

$$\Phi(\tilde{J})-\Phi(\tilde{J}_0)=t\ , \tag{6.22}$$

$$\Phi(\tilde{J})\equiv-\frac{1}{\alpha_2\tilde{J}}-\frac{\alpha_3}{\alpha_2^2}\ln\tilde{J}+O(\tilde{J})\ ,$$

which can be solved iteratively to get

$$\tilde{J}(t)=\tilde{J}_0\left[1-\alpha_2\tilde{J}_0t+\frac{\alpha_3}{\alpha_2^2}\tilde{J}_0\ln(1-\alpha_2\tilde{J}_0t)\right]^{-1}\ . \tag{6.23}$$

The result for $\tilde{J}(t)$ is equivalent to summing specific infinite subsets of terms in the perturbation series expressing $J(t)$ in powers of $\tilde{J}_0$. Indeed, the general expression relating $\tilde{J}(t)$ to $\tilde{J}_0$ can be expected to have the form

$$\begin{aligned}\tilde{J}(t)&=\tilde{J}_0+\sum_{m=2}^{\infty}A_m(t)\tilde{J}_0^m\\&=\tilde{J}_0+\sum_{m=2}^{\infty}\sum_{n=1}^{m}A_{m,n}t^{m-n}\tilde{J}_0^m\ .\end{aligned} \tag{6.24}$$

Then, deriving the recursion relation (6.21) up to order $\tilde{J}^r$ and integrating the result to obtain $\tilde{J}(t)$ in terms of $\tilde{J}_0$ is equivalent to summing up the infinite subset of terms in (6.23) that include all the coefficients up to $A_{m,r-1}$ for all

m. The labor involved in calculating $\alpha_1, \ldots, \alpha_r$ is little more than in doing perturbation theory up to rth order. Hence it is clear that, as long as the dimensionless couplings remain small, setting up and solving the perturbative scaling relations permit one to improve upon naive perturbation theory considerably without very much extra labor.

Second, consider the calculation of physical thermodynamic quantities at a temperature T, such as the free energy, or the magnetic susceptibility, etc., which will be denoted by F. As emphasized in Sec. V, this is best done in terms of $\widetilde{\mathscr{H}}_{\text{eff}}(t)$ [obtained by evaluating $\widetilde{\mathscr{H}}(D)$ at $D \cong 10T$]. By the arguments made earlier it is clear that in the present problem $\widetilde{\mathscr{H}}(D)$ has a good expansion in powers of $\widetilde{J}_{\text{eff}}(T)$ [obtained by evaluating $\widetilde{J}(D,T)$ at $D = 10T$] as long as T is in the local moment regime, i.e., $\widetilde{J}_{\text{eff}}(t)$ is small. Hence one expects to obtain a good expansion for F in powers of $\widetilde{J}_{\text{eff}}$. It is convenient to write this in the following form:

$$F = \phi_0 + \phi_1(\widetilde{J}_{\text{eff}} + \phi_2 \widetilde{J}^2_{\text{eff}} + \phi_3 \widetilde{J}^3_{\text{eff}} + \cdots) \equiv \phi_0 + \phi_1 \widetilde{F} \ . \tag{6.25}$$

Now consider calculating the perturbation series for $\widetilde{F}$ in powers of J_0. It will be of the form

$$\widetilde{F}(t) = \widetilde{J}_0 + \sum_{m=2}^{\infty} f_m(t) \widetilde{J}_0^m \tag{6.26a}$$

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{m} f_{m,n} t^{m-n} \widetilde{J}_0^m \ . \tag{6.26b}$$

The important point is that knowing $f_m(t)$ in (6.26a) up to $m=r$ permits one to evaluate ϕ_m in (6.25) up to $m=r$ by substituting the bad expansion for $\widetilde{J}_0$ in powers of $\widetilde{J}_{\text{eff}}$ up to order r in (6.26a). And this is equivalent to summing the infinite subset of terms in (6.26b) that include all coefficients up to $f_{m,r}$, resulting once again in a considerable improvement of perturbation theory.

Third, as is well known, the above results imply scaling laws and universality. From (6.22) it is clear that $\widetilde{J}_{\text{eff}}(T)$ can be written

$$\Phi(\widetilde{J}_{\text{eff}}(T)) = \ln(T_K/T) \ ,$$

where (6.27)

$$T_K \equiv (D_0/10) \exp[\Phi(\widetilde{J}_0)] \ .$$

Thus $\widetilde{J}_{\text{eff}}(T)$, and hence *all thermodynamic properties of the system,* can be expressed as a function only of T/T_K, and their dependence on the initial coupling constant $\widetilde{J}_0$, etc., enter only through the scaling temperature T_K, called the Kondo temperature. Note further that the scaling law continues to remain valid even when T gets small enough that $\mathscr{H}_{\text{eff}}(T)$ is no longer in the local moment regime and $\widetilde{J}_{\text{eff}}(T)$ has no meaning. This has been verified in the case when $\widetilde{J}_0$ is antiferromagnetic [whence $|\widetilde{J}_{\text{eff}}(T)|$ increases as T decreases and becomes of order unity when $T \cong T_K$] by Wilson[8] with the use of numerical RGT methods to trace the entire trajectory of $\mathscr{H}_{\text{eff}}(T)$. In the ferromagnetic case the effective coupling decreases as T decreases, and in this case the perturbative scaling procedure itself is enough to calculate all the thermodynamic properties.

Finally, we comment on the fact that the second- and third-order coefficients α_2 and α_3 in the recursion relation (6.21) can be obtained in two other ways: The first way is to note that since $\widetilde{F}$ has a good expansion in powers of $\widetilde{J}_{\text{eff}}(t)$ [$t \equiv \ln(D_0/10T)$ below] one can obtain a good expansion for $d\widetilde{F}/dt$ using (6.25):

$$\frac{d\widetilde{F}}{dt} = (1 + 2\phi_2 \widetilde{J}_{\text{eff}} + 3\phi_3 \widetilde{J}^2_{\text{eff}}) \frac{d\widetilde{J}_{\text{eff}}}{dt}$$

$$= \alpha_2 \widetilde{J}^2_{\text{eff}} + (\alpha_3 + 2\alpha_2\phi_2) \widetilde{J}^3_{\text{eff}}$$

$$+ (\alpha_4 + 2\alpha_3\phi_2 + 3\alpha_2\phi_3) \widetilde{J}^4_{\text{eff}} + \cdots \ . \tag{6.28}$$

Now one can invert (6.25) to express $\widetilde{J}_{\text{eff}}$ in terms of $\widetilde{F}$, and substitute in (6.28) to obtain a recursion relation for $\widetilde{F}$:

$$\frac{d\widetilde{F}}{dt} = \alpha_2 \widetilde{F}^2 + \alpha_3 \widetilde{F}^3 + [\alpha_4 - \alpha_3\phi_2 + \alpha_2(\phi_3 - \phi_2^2)] \widetilde{F}^4 \ . \tag{6.29}$$

The first two coefficients are identical to the coefficients in the recursion relation for $\widetilde{J}_{\text{eff}}(T)$. Hence an alternative way to obtain them is by using the procedure adopted to derive (6.21) with any thermodynamic property which has an expansion in powers of $\widetilde{J}_0$ starting with the linear term. Had this been done for F, one would have obtained [compare (6.17a), (6.26a), and (6.20)]

$$\frac{d\widetilde{F}}{dt} = f_2' \widetilde{F}^2 + [f_3'(t) - 2f_2(t) f_2'] \widetilde{F}^3 + \cdots \ . \tag{6.30a}$$

Thus one must have

$$f_2' = \alpha_2, \quad f_3' - 2f_2(t) f_2' = \alpha_3 \ . \tag{6.30b}$$

The second alternative way to derive α_2 and α_3 is by determining how one can compensate a small change in the cutoff D_0 by a suitable change in $\widetilde{J}_0$ so as to keep $\widetilde{F}$ invariant. Suppose that as $D_0 \rightarrow D_0 + dD_0$, $t \rightarrow t + dt$ and $\widetilde{J}_0 \rightarrow \widetilde{J}_0 + d\widetilde{J}_0$. From (6.26a) the condition is clearly that

$$d\widetilde{F} = d\widetilde{J}_0[1 + 2f_2(t)\widetilde{J}_0 + 3f_3(t)\widetilde{J}_0^2 + \cdots]$$

$$+ dt[f_2' \widetilde{J}_0^2 + f_3' \widetilde{J}_0^3 + \cdots] = 0 \ , \tag{6.31a}$$

whereupon

$$\frac{d\widetilde{J}_0}{dt} = f_2' \widetilde{J}_0^2 + (f_3' - 2f_2 f_2') \widetilde{J}_0^3 + \cdots \ . \tag{6.31b}$$

Comparing with (6.30a) and (6.30b) one notes that the first two coefficients of this expansion also correctly give α_2 and α_3.

It must be emphasized that the coefficients of the fourth-order terms in the "recursion relations" (6.21), (6.29), and (6.31b) will not, in general, be the same. The fact that the second- and third-order coefficients are the same depends entirely on the question of good expansion. This has not always been stressed in the literature, except by Wilson.

When the initial Hamiltonian is more complicated than the Kondo Hamiltonian, in general there will be several marginal variables, and perhaps relevant variables, in the problem. Even in such cases, one expects that a discussion similar in spirit to the one presented here, but different in detail, will be possible in each of the regimes of the fixed points.

VII. CONCLUDING REMARKS

We have found the thermodynamic scaling techniques developed in this paper to be of considerable value in analyzing two-impurity problems. In particular, we have used the techniques to study the two-impurity Kondo problem[13] and the two-impurity Anderson model[27] (especially in the mixed-valence regime). These studies will be discussed in detail elsewhere.

Furthermore, we envisage that the scaling techniques will be useful for calculating other static properties, e.g., spin correlations in the Kondo problem. The promise of the method lies in the possibility of using it in conjunction with nonperturbative RG techniques to study more realistic models of magnetic impurities in nonmagnetic metals. This will be especially true if one can learn to set up perturbative scaling equations with $\mathscr{U}$, and perhaps with some parts of $\mathscr{H}_I$, treated exactly as part of $\mathscr{H}_0$. Even more attractive is the possibility of extending the scaling method discussed in this paper to include dynamic properties. All these questions are being investigated.

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APPENDIX A: DERIVATION OF THE PERTURBATION EXPANSION FOR THE PARTITION FUNCTION Z

In this appendix we present a proof that the perturbation expansion for Z is given by (3.4), i.e.,

$$Z = \mathrm{Tr}\, e^{-\beta(\mathscr{H}_0+\mathscr{H}_I)}$$
$$= Z^{(0)} + Z^{(1)} + Z^{(2)} + \cdots , \tag{A1a}$$

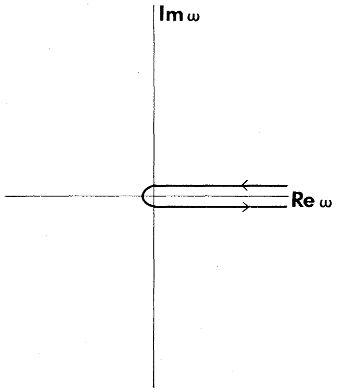

FIG. 1. Contour in the complex ω plane for the integral in Appendix A, Eq. (A2).

$$Z^{(0)} = \sum_j e^{-\beta E_j} , \tag{A1b}$$

$$Z^{(n)} = -\frac{\beta}{n} \sum_{j_1,\ldots,j_n} \langle j_1 | \mathscr{H}_I | j_2 \rangle \cdots \langle j_n | \mathscr{H}_I | j_1 \rangle \times \left[\sum_{i=1}^{n} e^{-\beta E_{j_i}} \left[\prod_{k\neq i} \frac{1}{E_{j_i} - E_{j_k}} \right] \right] , \tag{A1c}$$

where $| j_i \rangle$ is an eigenstate of $\mathscr{H}_0$ with eigenvalue E_{j_i}.

Consider the Laplace transform representation of $e^{-\beta\mathscr{H}}$,

$$e^{-\beta\mathscr{H}} = \int_C \frac{d\omega}{2\pi i} e^{-\beta\omega} \frac{1}{\omega - \mathscr{H}} , \tag{A2}$$

where C is the contour in the complex ω plane indicated in Fig. 1. Therefore,

$$Z = \mathrm{Tr}\, e^{-\beta\mathscr{H}} = \int_C \frac{d\omega}{2\pi i} e^{-\beta\omega} \sum_j \left\langle j \left| \frac{1}{\omega - \mathscr{H}} \right| j \right\rangle , \tag{A3}$$

where $\{ | j \rangle \}$ is the complete set of eigenstates of $\mathscr{H}_0$. Now one can obtain the perturbation expansion for Z by using the operator identity

$$\frac{1}{\omega - (\mathscr{H}_0 + \mathscr{H}_I)} = \frac{1}{\omega - \mathscr{H}_0} + \frac{1}{\omega - \mathscr{H}_0} \mathscr{H}_I \frac{1}{\omega - \mathscr{H}_0} + \cdots \tag{A4}$$

in (A3). The first term in (A4) gives $Z^{(0)}$ as given by (A1b). The nth-order term in (A4) gives, for $Z^{(n)}$,

$$Z^{(n)} = \int_C \frac{d\omega}{2\pi i} e^{-\beta\omega} \sum_j \left\langle j \left| \frac{1}{\omega - \mathscr{H}_0} \mathscr{H}_I \frac{1}{\omega - \mathscr{H}_0} \mathscr{H}_I \cdots \mathscr{H}_I \frac{1}{\omega - \mathscr{H}_0} \right| j \right\rangle , \tag{A5}$$

where $\mathscr{H}_I$ occurs n times. Introducing n sets of intermediate states $\{ | j_i \rangle \}$ appropriately into (A5), one gets

$$Z^{(n)} = \int_C \frac{d\omega}{2\pi i} e^{-\beta\omega} \sum_{j,j_1,\ldots,j_n} \left\langle j \left| \frac{1}{\omega - \mathscr{H}_0} \right| j_1 \right\rangle \left\langle j_1 \left| \mathscr{H}_I \frac{1}{\omega - \mathscr{H}_0} \right| j_2 \right\rangle \cdots \left\langle j_n \left| \mathscr{H}_I \frac{1}{\omega - \mathscr{H}_0} \right| j \right\rangle . \tag{A6}$$

Since $|j_i\rangle$ are eigenstates of $\mathcal{H}_0$ with eigenvalues E_{j_i}, Eq. (A6) can be simplified to read

$$Z^{(n)}=\sum_{j_1,\ldots,j_n}\langle j_1|\mathcal{H}_I|j_2\rangle\cdots\langle j_n|\mathcal{H}_I|j_1\rangle\int_C\frac{d\omega}{2\pi i}e^{-\beta\omega}\frac{1}{(\omega-E_{j_1})^2}\frac{1}{\omega-E_{j_2}}\cdots\frac{1}{\omega-E_{j_n}}\;. \tag{A7}$$

By symmetrizing (A7) with respect to all the $|j_i\rangle$, one gets

$$Z^{(n)}=-\frac{1}{n}\sum_{j_1,\ldots,j_n}\langle j_1|\mathcal{H}_I|j_2\rangle\cdots\langle j_n|\mathcal{H}_I|j_1\rangle\int_C\frac{d\omega}{2\pi i}e^{-\beta\omega}\frac{\partial}{\partial\omega}\left[\prod_{i=1}^{n}\frac{1}{\omega-E_{j_i}}\right], \tag{A8}$$

where $1/n$ compensates for the n equal terms that arise from the differentiation with respect to ω. Now (A8) can be integrated by parts; the contributions from the ends of the contour C vanish and one is left with

$$Z^{(n)}=-\frac{\beta}{n}\sum_{j_1,\ldots,j_n}\langle j_1|\mathcal{H}_I|j_2\rangle\cdots\langle j_n|\mathcal{H}_I|j_1\rangle\int_C\frac{d\omega}{2\pi i}e^{-\beta\omega}\left[\prod_{i=1}^{n}\frac{1}{\omega-E_{j_i}}\right]. \tag{A9}$$

(A9) is trivially evaluated by distorting the contour C to pick up the contributions due to each of the poles at $\omega=E_{j_i}$ and the result is nothing but (A1).

APPENDIX B: DETAILS OF THE DERIVATION OF THE RECURSION RELATIONS (3.3c) AND (3.3d)

The conditions on $\mathcal{H}_I^{(2)}(D)$ and $\mathcal{H}_I^{(3)}(D)$ obtained by the procedure described in Sec. III are given by

$$-\beta\sum_p\langle p|\mathcal{H}_I^{(2)}(D)|p\rangle e^{-\beta E_p}=-\beta\sum_{p,q}\langle p|\mathcal{H}_I|q\rangle\langle q|\mathcal{H}_I|p\rangle\left[\frac{e^{-\beta E_p}-e^{-\beta E_q}}{E_p-E_q}\right] \tag{B1}$$

and

$$\begin{aligned}-\beta\sum_p\langle p|\mathcal{H}_I^{(3)}(D)|p\rangle e^{-\beta E_p}-\frac{\beta}{2}\Bigg[&\sum_{p_1,p_2}[\langle p_1|\mathcal{H}_I^{(1)}(D)|p_2\rangle\langle p_2|\mathcal{H}_I^{(2)}(D)|p_1\rangle\\&+\langle p_1|\mathcal{H}_I^{(2)}(D)|p_2\rangle\langle p_2|\mathcal{H}_I^{(1)}(D)|p_1\rangle]\frac{e^{-\beta E_{p_1}}-e^{-\beta E_{p_2}}}{E_{p_1}-E_{p_2}}\Bigg]\\=-\beta\Bigg[&\sum_{p_1,p_2,q}\langle q|\mathcal{H}_I|p_1\rangle\langle p_1|\mathcal{H}_I|p_2\rangle\langle p_2|\mathcal{H}_I|q\rangle\left[\frac{e^{-\beta E_{p_1}}-e^{-\beta E_q}}{(E_{p_1}-E_q)(E_{p_1}-E_{p_2})}+(p_1\leftrightarrow p_2)\right]\\&+\sum_{p,q_1,q_2}\langle p|\mathcal{H}_I|q_1\rangle\langle q_1|\mathcal{H}_I|q_2\rangle\langle q_2|\mathcal{H}_1|p\rangle\left[\frac{e^{-\beta E_p}-e^{-\beta E_{q_1}}}{(E_p-E_{q_1})(E_{q_1}-E_{q_2})}+(q_1\leftrightarrow q_2)\right]\Bigg].\end{aligned} \tag{B2}$$

Equation (B1) is obtained by comparing the second-order term in the expansion for (3.6) with $Z^{(2)}$ given by (3.5c) while (B2) is obtained by comparing the third-order term of (3.6) with $Z^{(3)}$ given by (3.5d). In obtaining these the choice (3.3b) that $\mathcal{H}_I^{(1)}(D)=P\mathcal{H}_IP$ has already been used to cancel some terms, as noted in Sec. III.

The simplest way to satisfy (B1) is to choose

$$\langle p|\mathcal{H}_I^{(2)}(D)|p\rangle=-\sum_q\langle p|\mathcal{H}_I|q\rangle\langle q|\mathcal{H}_I|p\rangle\left[\frac{1-e^{-\beta(E_q-E_p)}}{E_q-E_p}\right]. \tag{B3}$$

Note that this determines only the diagonal elements of $\mathcal{H}_I^{(2)}(D)$, the operator itself can be of the general form

$$\mathcal{H}_I^{(2)}(D)=\sum_q(P_a\mathcal{H}_I|q\rangle\langle q|\mathcal{H}_IP_b)h^{(2)}(E_a,E_b;E_q) \tag{B4}$$

as long as $h^{(2)}(E_a,E_b;E_q)$ is symmetric when $E_a\leftrightarrow E_b$ and satisfies

$$h^{(2)}(E_a,E_a;E_q)=-\frac{1-e^{-\beta(E_q-E_a)}}{E_q-E_a}\;. \tag{B5}$$

The expression (3.3c) for $\mathcal{H}_I^{(2)}(D)$ corresponds to the obvious choice

$$h^{(2)}(E_a,E_b;E_q)=-\frac{1}{2}\left[\frac{1-e^{-\beta(E_q-E_a)}}{E_q-E_a}+\frac{1-e^{-\beta(E_q-E_b)}}{E_q-E_b}\right]. \tag{B6}$$

Note that the specific choice one makes for the off-diagonal part of $\mathcal{H}_I^{(2)}(D)$ influences the condition on the diagonal part $\mathcal{H}_I^{(3)}(D)$ via Eq. (B2).

By substituting the choices already made for $\mathcal{H}_I^{(1)}(D)$ and $\mathcal{H}_I^{(2)}(D)$ into (B2) and simplifying, one gets

$$\begin{aligned}\sum_p \langle p|\mathcal{H}_I^{(3)}(D)|p\rangle e^{-\beta E_p} = {} & \sum_{p,q_1,q_2} \langle p|\mathcal{H}_I|q_1\rangle\langle q_1|\mathcal{H}_I|q_2\rangle\langle q_2|\mathcal{H}_I|p\rangle \left[\frac{e^{-\beta E_p}-e^{-\beta E_{q_1}}}{(E_p-E_{q_1})(E_{q_1}-E_{q_2})}+(q_1\leftrightarrow q_2)\right]\\ & +\sum_{p_1,p_2,q}\langle q|\mathcal{H}_I|p_1\rangle\langle p_1|\mathcal{H}_I|p_2\rangle\langle p_2|\mathcal{H}_I|q\rangle\frac{1}{2}\frac{e^{-\beta E_{p_1}}+e^{-\beta E_{p_2}}}{(E_{p_1}-E_{p_2})}\\ & \times\left[\frac{1-e^{-\beta(E_q-E_{p_1})}}{(E_{p_1}-E_q)}-(p_1\leftrightarrow p_2)\right]. \end{aligned} \tag{B7}$$

Note that the choice for $\mathcal{H}_I^{(2)}(D)$ influences only the second term in (B7). It does not seem to be possible to choose it in such a way as to get rid of this term.

A simple way to ensure (B7) is to choose

$$\begin{aligned}\langle p|\mathcal{H}_I^{(3)}(D)|p\rangle = {} & \sum_{q_1,q_2}\langle p|\mathcal{H}_I|q_1\rangle\langle q_1|\mathcal{H}_I|q_2\rangle\langle q_2|\mathcal{H}_I|p\rangle\left[\frac{1-e^{-\beta(E_{q_1}-E_p)}}{(E_p-E_{q_1})(E_{q_1}-E_{q_2})}+(q_1\leftrightarrow q_2)\right]\\ & +\tfrac{1}{2}\sum_{p_1,q}(\langle p|\mathcal{H}_I|p_1\rangle\langle p_1|\mathcal{H}_I|q\rangle\langle q|\mathcal{H}_I|p\rangle+\text{H.c.})\\ & \times\frac{1}{(E_p-E_{p_1})}\left[\frac{1-e^{-\beta(E_q-E_p)}}{(E_p-E_q)}-(p\to p_1)\right]. \end{aligned} \tag{B8}$$

But (B8) still fixes only the diagonal elements. $\mathcal{H}_I^{(3)}(D)$ itself can be of the general form

$$\begin{aligned}\mathcal{H}_I^{(3)}(D)= {} & \sum_{a,b,q_1,q_2}(P_a\mathcal{H}_I|q_1\rangle\langle q_1|\mathcal{H}_I|q_2\rangle\langle q_2|\mathcal{H}_I P_b)h_1^{(3)}(E_a,E_b;E_{q_1},E_{q_2})\\ & +\frac{1}{2}\sum_{a,b,p,q}(P_a\mathcal{H}_I|p\rangle\langle p|\mathcal{H}_I|q\rangle\langle q|\mathcal{H}_I P_b+\text{H.c.})h_2^{(3)}(E_a,E_b;E_p,E_q), \end{aligned} \tag{B9}$$

and (B8) is satisfied as long as one ensures that

$$h_1^{(3)}(E_a,E_a;E_{q_1},E_{q_2})=\left[\frac{1-e^{-\beta(E_{q_1}-E_a)}}{(E_a-E_{q_1})(E_{q_1}-E_{q_2})}+(q_1\leftrightarrow q_2)\right], \tag{B10a}$$

$$h_2^{(3)}(E_a,E_a;E_p,E_q)=\frac{1}{(E_a-E_p)}\left[\frac{1-e^{-\beta(E_q-E_a)}}{(E_a-E_q)}-(a\to p)\right], \tag{B10b}$$

and provided $h_1^{(3)}(E_a,E_b;E_{q_1},E_{q_2})$ is symmetric under the interchange of E_a with E_b and E_{q_1} with E_{q_2}. The specific expression (3.3d) for $\mathcal{H}_I^{(3)}(D)$ corresponds to the choice

$$h_1^{(3)}(E_a,E_b;E_{q_1},E_{q_2})=\frac{1}{4}\left[\frac{1-e^{-\beta(E_{q_1}-E_a)}}{E_{q_1}-E_a}+(a\leftrightarrow b)\right](q_1\leftrightarrow q_2), \tag{B11a}$$

$$h_2^{(3)}(E_a,E_b;E_p,E_q)=\frac{1}{2}\left[\frac{1-e^{-\beta(E_p-E_a)}}{(E_p-E_a)}+(a\leftrightarrow b)\right]\left[\frac{1-e^{-\beta(E_q-E_a)}}{(E_q-E_a)}-(a\to p)\right]. \tag{B11b}$$

Note that while (B11b) satisfies (B10b), (B11a) reproduces (B10a) only up to terms of order $\exp(-D/T)$, which is admissible. The particular choice (B11) has been guided by the important requirement that the recursion relation (B4) and (B9) [or (3.3)] connecting $\mathscr{H}_I(D)$ to $\mathscr{H}_I$ must satisfy the semigroup property. We discuss this aspect next.

Let $D' < D < D_0$. Then a direct scaling transformation reducing the band edge from D_0 to D' leads to $\mathscr{H}_I(D')$ given by

$$\mathscr{H}_I^{(1)}(D') = P'\mathscr{H}_I P' \ , \tag{B12a}$$

$$\mathscr{H}_I^{(2)}(D') = \sum_{a,b,q'} (P'_a \mathscr{H}_I \,|\, q'\rangle\langle q' \,|\, \mathscr{H}_I P'_b) h^{(2)}(E_a,E_b;E_{q'}) \ , \tag{B12b}$$

$$\begin{aligned}\mathscr{H}_I^{(3)}(D') = &\sum_{a,b,q'_1,q'_2} (P'_a \mathscr{H}_I \,|\, q'_1\rangle\langle q'_1 \,|\, \mathscr{H}_I \,|\, q'_2\rangle\langle q'_2 \,|\, \mathscr{H}_I P'_b) h_1^{(3)}(E_a,E_b;E_{q'_1},E_{q'_2}) \\ &+\tfrac{1}{2} \sum_{a',b',p',q'} (P'_a \mathscr{H}_I \,|\, p'\rangle\langle p' \,|\, \mathscr{H}_I \,|\, q'\rangle\langle q' \,|\, \mathscr{H}_I P'_b + \text{H.c.}) h_2^{(3)}(E_a,E_b;E_{p'},E_{q'}) \ , \end{aligned} \tag{B12c}$$

where $|a\rangle, |b\rangle, |p'\rangle$ belong to P' and $|q'_1\rangle, |q'_2\rangle, |q'\rangle$ belong to Q' such that P' contains no electrons and holes of energy between D' and D_0 and Q' contains at least one electron or hole of energy between D' and D_0.

But $\mathscr{H}_I(D')$ can also be obtained by two successive applications of the scaling transformation: First by reducing the cutoff from D_0 to D so as to obtain $\mathscr{H}_I(D)$ as given by (3.3), then by reducing the cutoff from D to D' to obtain $\mathscr{H}_I(D')$ in terms of $\mathscr{H}_I(D)$. The requirement of the semigroup property is that the result must agree order by order with that obtained by (B12).

Let R denote the subspace of states with no electrons or holes of energy above D, but with at least one electron or hole of energy between D' and D. Then $\mathscr{H}_I(D')$ obtained by the two successive transformations can be obtained in terms of $\mathscr{H}_I(D)$ by replacing $\mathscr{H}_I$ by $\mathscr{H}_I(D)$ and $\{|q'_1\rangle, |q'_2\rangle, |q'\rangle\}$ by $\{|r_1\rangle, |r_2\rangle, |r\rangle\} \in R$. Collecting together the various orders of $\mathscr{H}_I(D')$ so obtained, one gets

$$\mathscr{H}_I(D') = P'\mathscr{H}_I^{(1)}(D) P' \ , \tag{B13a}$$

$$\mathscr{H}_I(D') = P'\mathscr{H}_I^{(2)}(D) P' + \left[\sum_{a,b,r} P'_a \mathscr{H}_I^{(1)}(D) \,|\, r\rangle\langle r \,|\, \mathscr{H}_I^{(1)} P'_b h^{(2)}(E_a,E_b;E_r) \right] , \tag{B13b}$$

$$\begin{aligned}\mathscr{H}_I^{(3)}(D) = P'\mathscr{H}_I^{(3)}(D) + &\left[\sum_{a,b,r} [P'_a \mathscr{H}_I^{(1)}(D) \,|\, r\rangle\langle r \,|\, \mathscr{H}_I^{(2)}(D) P'_b + P'_a \mathscr{H}_I^{(2)}(D) \,|\, r\rangle\langle r \,|\, \mathscr{H}_I^{(1)}(D) P'_b] h^{(2)}(E_a,E_b;E_r) \right] \\ + &\left[\sum_{a,b,r_1,r_2} [P'_a \mathscr{H}_I^{(1)}(D) \,|\, r_1\rangle\langle r_1 \,|\, \mathscr{H}_I^{(1)}(D) \,|\, r_2\rangle\langle r_2 \,|\, \mathscr{H}_I^{(1)}(D) P'_b] h_1^{(3)}(E_a,E_b;E_{r_1},E_{r_2}) \right. \\ &\left. +\tfrac{1}{2} \sum_{a,b,p',r} [P'_a \mathscr{H}_I^{(1)}(D) \,|\, p'\rangle\langle p' \,|\, \mathscr{H}_I^{(1)}(D) \,|\, r\rangle\langle r \,|\, \mathscr{H}_I^{(1)}(D) P'_b + \text{H.c.}] h_2^{(3)}(E_a,E_b;E_{p'},E_r) \right] . \end{aligned} \tag{B13c}$$

The requirement of the semigroup property is equivalent to the demand that the results obtained by substituting for $\mathscr{H}_I(D)$ in terms of $\mathscr{H}_I$ in (B13) must agree with (B12).

It is evident that (B13a) with $\mathscr{H}_I^{(1)}(D)$ being given by (3.3b) is consistent with (B12a) since P' is a subset of P. In order to compare (B13b) with (B12b), one makes use of the expression (B4) for $\mathscr{H}_I^{(2)}(D)$ and notes that R is also a subset of P and that

$$Q + R = Q', \text{ i.e., } \sum_q + \sum_r = \sum_{q'} \ . \tag{B14}$$

Hence it follows that (B13b) agrees with (B12b) for arbitrary choices of $h^{(2)}$.

Next consider the comparison of (B13c) with (B12c). The easiest way to make the comparison is to substitute for $\mathscr{H}_I^{(3)}(D)$ and $\mathscr{H}_I^{(2)}(D)$ from (B9) and (B4), respectively, in (B13c), and to replace $\sum_q + \sum_r$ by $\sum_{q'}$. Similarly replace $\sum_{p'}$ by $\sum_p - \sum_r$ in (B12c), and then compare the resulting expressions. It is then a matter of straightforward, albeit tedious algebra to show that they agree, provided that

$$h_1^{(3)}(E_a,E_b;E_r,E_q) = \tfrac{1}{2} h_2^{(3)}(E_a,E_b;E_r,E_q) + h^{(2)}(E_a,E_b;E_r) h^{(2)}(E_r,E_b;E_q) \tag{B15}$$

It is important to note that, since terms of order $e^{-D/T}$ and $e^{-D'/T}$ have been neglected in deriving the expressions for $\mathscr{H}_I(D)$ and $\mathscr{H}_I(D')$, one can only demand that (B15) be satisfied up to terms of order $e^{-\beta(E_q - E_a)}$, etc. $h^{(2)}$, as given by (B6), and $h_1^{(3)}$ and $h_2^{(3)}$, as given by (B11), are the simplest we have been able to find that meet the above demands. Clearly, other possibilities are not ruled out.

APPENDIX C: EVALUATION OF THE COEFFICIENTS IN EQ. (6.21)

Recall that

$$\alpha_3 = A'_3(t) - 2A_2(t)A'_2 \ , \tag{C1}$$

where $A_3(t)$ and $A_2(t)$ are given by (6.17). One has

$$A_2(t) = -t, \quad A'_2 = -1 \ , \tag{C2a}$$

$$A_3'(t)=\tfrac{1}{2}\{\,2t[S(S+1)+1]-1 \\ -[2I_1'(t)-I_2'(t)][S(S+1)-1] \\ +I_3'(t)[S(S+1)+1]\}\ , \tag{C2b}$$

where $I_1(t)$, $I_2(t)$, and $I_3(t)$ are given by (6.7) with the substitution $D=D_0e^{-t}$.

First consider $I_1'(t)$ and $I_2'(t)$. It is easy to verify that by rescaling the integration variable q one can write

$$I_1(t)=\int_{e^{-t}}^{1}\frac{dq}{q}\ln\left[\frac{1+q}{q}\right]\ ,$$
$$I_2(t)=\int_{1}^{e^{-t}}\frac{dq}{q}\ln\left[\frac{1+q}{q}\right]\ . \tag{C3}$$

Hence, we obtain

$$I_1'(t)=t+\ln(1+e^{-t})\ , \tag{C4a}$$
$$I_2'(t)=\ln(1+e^{-t})\ . \tag{C4b}$$

A careful evaluation of I_3' is more tedious. Recall that

$$I_3=\int_D^{D_0}\frac{dq}{q}I_4(q)\ , \tag{C5a}$$

where

$$I_4(q)=\int_0^D d\epsilon\left[\frac{e^{-\beta(q-\epsilon)}-1}{q-\epsilon}+e^{-\beta q}\left[\frac{e^{\beta\epsilon}-1}{\epsilon}\right]\right]\ . \tag{C5b}$$

I_4 can be evaluated in terms of exponential integral functions:

$$I_4(q)=e^{-\beta q}[\mathrm{Ei}(\beta\epsilon)-\ln(\beta\epsilon)]_0^D+[\ln(\beta(q-\epsilon))-\mathrm{Ei}(-\beta(q-\epsilon))]_0^D \\ =e^{-\beta q}[\mathrm{Ei}(\beta D)-\ln(\beta D)-\gamma]+[\ln(\beta(q-D))-\mathrm{Ei}(-\beta(q-D))-\ln(\beta q)+\mathrm{Ei}(-\beta q)]\ , \tag{C6}$$

where γ is Euler's constant. Hence one has

$$I_3'(t)=-D\frac{\partial I_3}{\partial D}=I_4(q=D)-D\int_D^{D_0}\frac{dq}{q}\frac{\partial I_4}{\partial D}(q)\ , \tag{C7a}$$

$$I_4(q=D)=e^{-\beta D}[\mathrm{Ei}(\beta D)-\ln(\beta D)-\gamma]+[\mathrm{Ei}(-\beta D)-\ln(\beta D)-\gamma]\ , \tag{C7b}$$

$$\frac{\partial I_4}{\partial D}(q)=e^{-\beta q}\left[\frac{e^{\beta D}}{D}-\frac{1}{D}\right]+\left[\frac{-1}{q-D}+\frac{e^{-\beta(q-D)}}{q-D}\right]=(e^{-\beta(q-D)}-1)\frac{q}{D(q-D)}+\frac{1-e^{-\beta q}}{D}\ , \tag{C7c}$$

so that

$$D\int_D^{D_0}\frac{dq}{q}\frac{\partial I_4}{\partial D}(q)=[\mathrm{Ei}(-\beta(D_0-D))-\ln(\beta(D_0-D))-\gamma] \\ +[\ln(\beta D_0)-\mathrm{Ei}(-\beta D_0)-\ln(\beta D)+\mathrm{Ei}(-\beta D)]\ . \tag{C7d}$$

Putting all the results together, noting that for large x,

$$\mathrm{Ei}(x)=\frac{e^x}{x}\left[1+\frac{1}{x}+\cdots\right]\ , \tag{C8}$$

and neglecting terms which are outright of order $e^{-\beta D}$, $e^{-\beta D_0}$, or $e^{-\beta(D_0-D)}$, one gets (with $D=D_0e^{-t}$)

$$I_3'(t)\cong e^{-\beta D}\mathrm{Ei}(\beta D)+\ln\left[1-\frac{D}{D_0}\right]-e^{-\beta D}\ln(\beta D)\ . \tag{C9}$$

Note that the first term is of order T/D, but the last term can be neglected. Substituting the results (C4) and (C9) into (C2b), one has

$$A_3'(t)=\tfrac{1}{2}\{4t-1+[S(S+1)+1][e^{-\beta D}\mathrm{Ei}(\beta D)+\ln(1-e^{-t})]-[S(S+1)-1][\ln(1+e^{-t})]\}\ , \tag{C10}$$

so that, if one neglects terms of order T/D and D/D_0, one indeed gets, as stated,

$$\alpha_3=(2t-\tfrac{1}{2})-2t=-\tfrac{1}{2}\ . \tag{C11}$$

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[14] For example, H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1003 (1980); **21**, 1043 (1980).

[15] This philosophy has been used adroitly to understand the nondegenerate Anderson model. See F. D. M. Haldane, Phys. Rev. Lett. **40**, 416 (1978); **40**, 911(E) (1978).

[16] For a precise statement about the conditions which permit this, see Sec. V.

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[20] We note that this approximation is mainly one of convenience. The neglected terms can be included at the expense of algebraic complication as an additional constant term in $H_1(D)$. But this is unnecessary, since, as will be shown later, it is sufficient to carry out the scaling down to $D \neq 10T$, whence the errors induced by the approximation are neglible.

[21] It is worth noting an important difference between the present recursion relations and the RG recursion relations encountered in classical statistical mechanics; the "unintegrated" degrees of freedom can enter as intermediate states. This is true of the second term in (3.3d) and of the terms listed in Table II. The difference is due to quantum mechanics.

[22] See C. Bloch, in *Studies in Statistical Mechanics,* edited by J. de Boer and G. E. Uhlenbeck (North-Holland, Amsterdam, 1965), Vol. III, p. 3; L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, New York, 1980), p. 95.

[23] In order that (5.7) may be considered RG equations, $\widetilde{\beta}_D$ must be regarded as a coupling constant; the scaling equation for this can be obtained easily from (5.8).

[24] Wilson's methods amount to the calculation of $H_{\text{eff}}(T_N)$ for a logarithmically discrete sequence of temperatures $T_N \sim \Lambda^{-N/2}D$, where Λ is a parameter greater than unity.

[25] See Ref. 8, Sec. V.

[26] These are scattered in the field theory and condensed-matter literature. See D. J. Gross, in *Methods in Field Theory,* edited by R. Balian and J. Zinn-Justin (North-Holland, Amsterdam, 1976), and Ref. 11.

[27] See C. Jayaprakash, H. R. Krishna-murthy, and J. W. Wilkins, J. Appl. Phys. (in press).