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# Spatially dependent zero-frequency response functions and correlation functions in the Kondo model

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We present the details of a formalism for calculating spatially varying zero-frequency response functions and equal-time correlation functions in models of magnetic and mixed-valence impurities of metals. The method is based on a combination of perturbative, thermodynamic scaling theory [H. R. Krishnamurthy and C. Jayaprakash, Phys. Rev. B **30**, 2806 (1984)] and a nonperturbative technique such as the Wilson renormalization group. We illustrate the formalism for the spin-$\frac{1}{2}$ Kondo problem and present results for the conduction-spin-density–impurity-spin correlation function and conduction-electron charge density near the impurity. We also discuss qualitative features that emerge from our calculations and discuss how they can be carried over to the case of realistic models for transition-metal impurities.

## I. INTRODUCTION

In an earlier paper[1] we introduced a formalism for calculating spatially dependent, zero-frequency response functions and equal-time correlation functions for a single magnetic impurity in a nonmagnetic metal. We calculated the response function measured in NMR Knight-shift experiments in dilute magnetic alloys and explained (from first principles) a significant feature of its behavior. The purpose of this paper is (i) to describe the details of the formalism and the calculation of the response function measured in the Knight-shift experiment and (ii) to present results for the conduction-electron-spin-density–impurity-spin correlation function and the conduction-electron charge density around the impurity.

We consider the spin-$\frac{1}{2}$ Kondo Hamiltonian

$$H_K(D_0)=H_c(D_0)-J_0\mathbf{s}(\mathbf{0})\cdot\mathbf{S}\ , \tag{1}$$

where $H_c(D_0)$ describes conduction electrons with a bandwidth of $2D_0$, $\mathbf{S}$ is the impurity spin at the origin, and $\mathbf{s}(\mathbf{0})$ $[=\psi_\mu^\dagger(0)(\frac{1}{2}\sigma_{\mu\nu})\psi_\nu(0)]$ is the conduction-electron spin density at the origin. In the preceding, $\psi_\mu^\dagger(\mathbf{r})$ denotes a creation operator for a conduction electron with spin $\mu$ at position $\mathbf{r}$. This model has been studied extensively and thermodynamic quantities such as the susceptibility $\chi(T)$ and the specific heat have been calculated exactly[2] for this and several related impurity models. Approximate (large-degeneracy-expansion) methods[3,4] have been successfully used to compute transport properties and spectral functions.[4] In contrast, spatially-varying properties have only been explored using perturbative methods until recently. Spatially varying correlation functions and zero-frequency response functions provide important probes of the many-particle state of the magnetic impurity system. Correlation functions such as the conduction-electron charge density at $\mathbf{r}$ given by $\langle\psi_\mu^\dagger(\mathbf{r})\psi_\mu(\mathbf{r})\rangle$, and the impurity-spin–conduction-electron spin-density correlation function $\langle\mathbf{S}\cdot\mathbf{s}(\mathbf{r})\rangle$ are clearly of interest. We will also consider $\langle\langle s_z(\mathbf{r});S_z\rangle\rangle_{H_K,\omega=0}$, where $\langle\langle A;B\rangle\rangle_{H,\omega=0}$ denotes the zero-frequency response function evaluated with the Hamiltonian $H$: $\langle\langle A;B\rangle\rangle_\omega$ is the Fourier transform of the retarded double-time Green's function[5]

$$\langle\langle A(t);B(0)\rangle\rangle_R=-i\Theta(t)\langle A(t)B(0)-B(0)A(t)\rangle\ , \tag{2}$$

where $A(t)$ and $B(0)$ are Heisenberg operators and

$$\langle(\cdots)\rangle\equiv\mathrm{Tr}[e^{-\beta H}(\cdots)]/\mathrm{Tr}e^{-\beta H}\ .$$

Indeed, some response functions can be measured directly. For example, consider NMR Knight-shift experiments in dilute magnetic alloys such as Cu-Fe.[6] The host NMR spectrum consists of a large, main resonance line due to host nuclei far from the impurity and weak satellite signals due to nuclei near the impurity. The satellites have their resonance field shifted from the main line, and this extra Knight shift $\Delta K(r,T)$ at a distance $r$ from the impurity essentially measures the conduction-electron spin-density response functions at the host nuclear position $r$. It can be shown that

$$\frac{\Delta K(r,T)}{K_0}=\frac{\langle\langle s_z(r);g_es_z+g_dS_z\rangle\rangle_{H_K,\omega=0}-\langle\langle s_z(r);g_es_z\rangle\rangle_{H_c,\omega=0}}{\langle\langle s_z(r);g_es_z\rangle\rangle_{H_c,\omega=0}}\ , \tag{3}$$

where, $K_0$ is the Knight shift of the pure metal described by the Hamiltonian $H_c$ and is proportional to the denominator on the right-hand side which is simply the Pauli susceptibility. The $g$ factors of the conduction-electron and impurity spins are denoted by $g_e$ and $g_d$, respectively. An interesting feature of the experiments is that the temperature dependence and $r$ dependence factorize. Our method show how this factorization arises, permits a detailed calculation of the spatial and temperature dependences of $\Delta K/K_0$, and provides an estimate of deviations from factorization. We emphasize that our method works only for $r$ such that $r \ll D_0/k_F T_K$ ("Kondo screening length"). This condition is easily satisfied with $k_F r \lesssim 10-15$ which is, however, sufficient for comparison with experiments. Recently, correlation functions have also been calculated using quantum Monte Carlo simulations[7] and small-$U$ expansion[8] in the symmetric Anderson model.

The rest of the paper is organized as follows. Section II discusses the general formalism, and introduces the perturbative, thermodynamic scaling method.[9] In Sec. III, we discuss the calculation of $\Delta K$ including the extension of Wilson's renormalization-group scheme[10] to the calculation of zero-frequency response functions. In Sec. IV, we present the results for $\langle \mathbf{S}\cdot\mathbf{s}(\mathbf{r})\rangle$ and $\langle \psi_\mu^\dagger(\mathbf{r})\psi_u(\mathbf{r})\rangle$. The extension to models with higher-spin impurities is addressed in Sec. V. Some algebraic details are relegated to the Appendices.

## II. GENERAL FORMALISM

We begin with a brief outline of the physical motivation of our method for obtaining the temperature dependence and $r$ dependence of zero-frequency response functions and correlation functions which we denote by $C(r,T)$ ($r$ is the distance from the impurity). The $r$ dependence (for $k_F r \ll D_0/T_K$, where $k_F$ is the Fermi wave vector) is determined essentially by the high energy (near the band edge) degrees of freedom since only those conduction electrons and holes can distinguish spatial separations of a few lattice spacings. This permits the spatial dependence to be determined by a perturbative scaling method. The temperature dependence, in contrast, is primarily due to low-energy degrees of freedom since $T \ll D_0$ the bandwidth. The difficulty in determining the $T$ dependence is associated with the well-known divergences of the Kondo problem and can be overcome by using the Wilson renormalization-group (RG) technique.

Motivated by the above observation, we employ the perturbative, thermodynamic scaling procedure to eliminate iteratively the high-energy electron and hole degrees of freedom; we emphasize that this procedure preserves the free energy. We reduce the bandwidth from $D_0$ to $D$, and generate an effective Hamiltonian $H(D)$ which describes the physics at lower-energy scales. Correlation functions evaluated with the original Hamiltonian with cutoff $D_0$, $H(D_0)$, become linear combinations of correlation functions evaluated with $H(D)$. When the bandwidth is $D$, the most localized state that can be formed at the origin by superposing conduction-electron plane-wave states has a spatial width approximately $\hbar v_F/D$, which is much larger than $r$ if $rD/\hbar v_F \ll 1$. Then, the $r$-dependent correlation functions evaluated with $H(D)$ reduce to *local* correlation functions. Thus, the correlation function of interest becomes a sum of terms which are products of functions of $r$ (essentially independent of $T$) and local correlation functions that involve operators with the same symmetry as $C(r,T)$. Thus, by choosing $D$ sufficiently small for a given $r$, the $r$-dependence can be extracted because precisely those high-energy degrees of freedom, which determine this dependence, have been integrated out. Note that, in order that our perturbative method remain accurate, $D$ must satisfy the condition that all dimensionless couplings are smaller than unity (in effect, the Kondo temperature $T_K$ and the temperature $T$, must be smaller than $D$). Thus, $D$ must be chosen such that $T, T_K \ll D \ll D_0/k_F r$, which is possible for experimentally interesting ranges of $k_F r$ and $T_K$. The local correlation functions evaluated with $H(D)$ determine the $T$ dependence and these are evaluated by using the Wilson RG method. Thus, by a judicious combination of perturbative and nonperturbative methods, $C(r,T)$ can be determined. Of course, the $r$ dependence, in practice, is determined only to leading order in perturbative scaling, and thus has limited accuracy (proportional to $\rho_0 J_0$ for small $\rho_0 J_0$). For a typical value $\rho_0 J_0 = -0.1$, the accuracy is about 10%.

Now we embark on a more detailed description of the calculation. Consider the evaluation of a general correlation function

$$\tilde{C}(\mathbf{r},T)=\langle \psi_\mu^\dagger(\mathbf{r})\mathcal{S}(\mu,\mu')\psi_{\mu'}(\mathbf{r})\rangle \ , \tag{4}$$

where $\mathcal{S}(\mu,\mu')$ is an operator in impurity space. For example, if $\mathcal{S}(\mu,\mu')=\frac{1}{2}\mathbf{S}\cdot\boldsymbol{\sigma}_{\mu\mu'}$, we have the conduction-electron-spin-density–impurity-spin correlation function. $S(\mu,\mu')=\delta_{\mu\mu'}$ yields the conduction-electron charge density at $\mathbf{r}$. For convenience, we will assume that the operator in the rhs of Eq. (4) is in normal-ordered form in terms of electron and hole operators (normal ordering here is equivalent to subtracting out a trivial constant). This correlation function can be evaluated by introducing an auxiliary field $\tilde{h}$ as follows.

Define the Hamiltonian

$$\tilde{H}(D_0)=H_K(D_0)-\tilde{h}\psi_\mu^\dagger(\mathbf{r})\mathcal{S}(\mu,\mu')\psi_{\mu'}(\mathbf{r}) \tag{5}$$

and the corresponding free energy

$$\tilde{F}=-k_B T \ln \mathrm{Tr} e^{-\beta \tilde{H}(D_0)} \ . \tag{6}$$

The required correlation function is given by

$$\tilde{C}(\mathbf{r},T)=-\frac{\partial}{\partial \tilde{h}}\tilde{F}\bigg|_{\tilde{h}=0} \ . \tag{7}$$

Similarly, a zero-frequency response function can be generated by introducing two auxiliary fields and using the second-derivative of the appropriate free energy in zero field (see Sec. III).

As discussed above, the first part of our procedure consists in reducing the bandwidth from $D_0$ to $D$ to extract the $r$ dependence. This is accomplished by using thermodynamic scaling theory, a finite-temperature formalism designed to handle *irrelevant* variables which are important for calculating spatial dependence of physical quantities. The formalism is an extension of a scaling method due to Anderson.[11] We now provide a brief review of the method to second order in the coupling constants which is sufficient for the work presented here. Details can be found in Ref. 9. We will first introduce the generalized impurity Hamiltonian $H$ which encompasses all the forms of Hamiltonians including the auxiliary-field terms needed in this paper. The conduction band of the metal is assumed to be isotropic with a density of states $\rho_0(\varepsilon)$ between $\pm D_0$ about the Fermi level. [We will choose $\rho_0(\varepsilon)=\rho_0$.] The conduction-electron states are labeled by $(\varepsilon\mu)$, where $\varepsilon$ is the energy and $\mu$ stands for other discrete or continuous labels, e.g., $\mu\equiv(\hat{\mathbf{k}}\alpha)$, where $\hat{\mathbf{k}}$ is the direction of the electron wave vector and $\alpha$ its spin. The corresponding creation operator, denoted by $c^\dagger_{\varepsilon\mu}$ obeys the anticommutation relation

$$\{c^\dagger_{\varepsilon\mu},c_{\varepsilon'\mu'}\}=\delta_{\mu\mu'}\delta(\varepsilon-\varepsilon')/\rho_0(\varepsilon) .$$

In this representation the conduction-electron Hamiltonian assumes the form

$$H_0=\int_{\varepsilon\mu}\varepsilon c^\dagger_{\varepsilon\mu}c_{\varepsilon\mu} ,$$

where $\int_{\varepsilon\mu}$ stands for $\sum_\mu\int d\varepsilon\,\rho_0(\varepsilon)$ and $\sum_\mu$ denotes appropriate sums and integrals [if $\mu\equiv(\hat{\mathbf{k}},\alpha)$, then $\sum_\mu=\sum_\alpha\int d\hat{\mathbf{k}}$]. The generalized impurity Hamiltonian can be written as

$$\begin{aligned} H&=H_0+H_I=H_0+H_{I1}+H_{I2}+\cdots ,\\ H_{I1}&=\mathcal{U} , \qquad (8)\\ H_{I2}&=\int_{\varepsilon\mu}\int_{\varepsilon'\mu'}c^\dagger_{\varepsilon\mu}c_{\varepsilon'\mu'}\mathcal{S}(\varepsilon\mu;\varepsilon'\mu') ,\end{aligned}$$

where $\mathcal{U}$ and $\mathcal{S}$ are operators in the finite-dimensional space of impurity states. For example, $H_K$ in Eq. (1) corresponds to

$$\mathcal{U}=0$$

and

$$\mathcal{S}(\varepsilon\alpha;\varepsilon'\alpha')=-\tfrac{1}{2}J_0\mathbf{S}\cdot\sigma_{\alpha\alpha'} .$$

The Hamiltonian is also assumed to be in the normal-ordered form in terms of electron and hole operators.[9] The scaling procedure is defined as follows: One "eliminates" the higher-energy scales, reducing the cutoff from $D_0$ to $D$, simutaneously changing the Hamiltonian from $H(D_0)$ to $H(D)$ so as to preserve the low-temperature properties of the system. The eigenstates of $H_0$ are divided into a set $\{|p\rangle\}$ which contains no electrons or holes of energy $D<\varepsilon<D_0$ and a complementary set $\{|q\rangle\}$, which contains at least one electron or hole of energy $D<\varepsilon<D_0$. The energy of the state $|q\rangle$, $E_0(q)$ is larger than $D$, and we will be interested in temperature $T\ll D<D_0$. Now consider the evaluation of $\mathrm{Tr}\,e^{-\beta(H_0+H_I)}$ in perturbation theory in $H_I$ where the trace is over all states. Neglecting terms of order $e^{-\beta E_0(q)}\ll1$, the partition function can be written as $\mathrm{Tr}_p e^{-\beta H(D)}$, where $\mathrm{Tr}_p$ denotes the trace over only $\{|p\rangle\}$. The states of the impurity are unaffected by the scaling procedure. When this procedure is applied to generalized impurity Hamiltonian $H$ given in Eq. (8), to second order in $H_I$, the Hamiltonian $H(D)$ can be represented in the same form; it is different from $H(D_0)$ in that $\mathcal{U}$ and $\mathcal{S}$ assume new "values" denoted by $\mathcal{U}_D$ and $\mathcal{S}_D$. Not only are the values of the original couplings renormalized but also different interaction terms that can be cast in the form in Eq. (8) are generated.

An important feature of this scaling method is that it can keep track of the energy dependences of the interactions in $\mathcal{U}_D$ and $\mathcal{S}_D$. Such terms, while irrelevant in the renormalization-group sense, are crucially important in calculating spatially dependent quantities such as $\tilde{C}(\mathbf{r},T)$. The simple reason is that 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 scaling procedure (i.e., until $D$ has been reduced sufficiently to neglect them).

Differential recursion relations can be obtained for the variation of $\mathcal{U}$ and $\rho$ with $D$ by scaling $D$ down to $D-\delta D$ to obtain $\mathcal{U}_{D-\delta D}$ and $\mathcal{S}_{D-\delta D}$. The general recursion relations are

$$\begin{aligned}\frac{d\mathcal{U}_D}{dD}=\int_{p\mu}\int_\varepsilon[&\mathcal{S}_D(-p\mu;D\nu)\mathcal{S}_D(D\nu;-p\mu)\\ &+\mathcal{S}_D(-D\nu;p\mu)\mathcal{S}_D(p\mu;-D\nu)]\frac{1}{D+p}\end{aligned} \tag{9}$$

and

$$\begin{aligned}\frac{d\mathcal{S}_D}{dD}=\tfrac{1}{2}\int_\nu\Bigg[&\mathcal{S}_D(\varepsilon\mu;D\nu)\mathcal{S}_D(D\nu;\varepsilon'\mu')\rho_0(D)\\ &\times\left[\frac{1-e^{-\beta(D-\varepsilon)}}{D-\varepsilon}+\frac{1-e^{-\beta(D-\varepsilon')}}{D-\varepsilon'}\right]\\ &+\mathcal{S}_D(-D\nu;\varepsilon'\mu')\mathcal{S}_D(\varepsilon\mu;-D\nu)\rho_0(-D)\\ &\times\left[\frac{1}{D+\varepsilon}+\frac{1}{D+\varepsilon'}\right]\Bigg] ,\end{aligned} \tag{10}$$

where $\int_{p\mu}$ stands for $\sum_\mu\int_0^D\rho_0(\pm p)dp$ as appropriate.

These recursion relations will be employed extensively in the rest of the paper. Their derivation can be found in Ref. 9. Now consider applying this method to $\tilde{H}(D_0)$ in Eq. (5). Perturbative scaling can be performed to reduce the cutoff from $D_0$ to $D$ so as to preserve the free energy to first order in $\tilde{h}$. This is sufficient since $\tilde{C}$ depends only on the first derivative of the free energy with respect to $\tilde{h}$ evaluated in zero field. In the course of the scaling procedure, new terms linear in $\tilde{h}$ are generated. The most general form of the effective Hamiltonian is given by

$$\begin{aligned}\tilde{H}(D)=H_K(D)-\tilde{h}\{&\psi^\dagger_\mu(\mathbf{r})\tilde{\mathcal{S}}_D(\mu\mu')\psi_{\mu'}(\mathbf{r})\\ &+[\psi^\dagger_\mu(\mathbf{r})\tilde{\mathcal{S}}'_D(\mu\mu')\psi_{\mu'}(0)+\mathrm{H.c.}]\\ &+\psi^\dagger_\mu(0)\tilde{\mathcal{S}}''_D(\mu,\mu')\psi_{\mu'}(0)\}-\tilde{h}\tilde{\mathcal{U}}_D ,\end{aligned} \tag{11}$$

where $\widetilde{\mathcal{S}}_D$, $\widetilde{\mathcal{S}}'_D$, $\widetilde{\mathcal{S}}''_D$, and $\widetilde{\mathcal{U}}_D$ are impurity operators with coefficients (or coupling constants) which are $r$ dependent.

Since the free energy is preserved we have

$$\widetilde{C}=\frac{\partial}{\partial\beta\widetilde{h}}\ln \mathrm{Tr}_{D_0} e^{-\beta\widetilde{H}(D_0)}=\frac{\partial}{\partial\beta\widetilde{h}}\ln \mathrm{Tr}_{D} e^{-\beta\widetilde{H}(D)} .$$

Therefore, $\widetilde{C}$ becomes a linear combination of correlation functions evaluated with $H_K(D)$ due to the terms linear in $\widetilde{h}$ present in Eq. (11):

$$\begin{aligned}\widetilde{C}=&\langle \psi^\dagger_\mu(\mathbf{r})\widetilde{\mathcal{S}}_D(\mu,\mu')\psi_{\mu'}(\mathbf{r})\rangle_{H_K(D)}\\&+\langle \psi^\dagger_\mu(\mathbf{r})\widetilde{\mathcal{S}}'_D(\mu,\mu')\psi_{\mu'}(0)\rangle_{H_K(D)}\\&+\langle \psi^\dagger_\mu(0)\widetilde{\mathcal{S}}''_D(\mu,\mu')\psi_{\mu'}(0)\rangle_{H_K(D)}+\langle \widetilde{\mathcal{U}}_D\rangle_{H_K(D)} .\end{aligned}\tag{12}$$

Assume that we can reduce the bandwidth from $D_0$ down to $D$ such that $rD/v_F \ll 1$. Then, a further simplification ensues: $\psi_\mu(\mathbf{r})$ can be replaced by $\psi_\mu(0)$. To see this, note that $H_K(D)$ is spherically symmetric; only in terms involving $s$-wave conduction electrons or holes can operators contribute to $\widetilde{C}$. To be specific, we expand $\psi_\mu(\mathbf{r})$ in terms of partial waves with respect to the origin:

$$\psi_\mu(\mathbf{r})=\int_\varepsilon\int_{\hat{\mathbf{k}}} e^{i\mathbf{k}\cdot\mathbf{r}}c_{\varepsilon\hat{\mathbf{k}}\mu}=\int_\varepsilon\int_{\hat{\mathbf{k}}}\sum_{l,m} Y_{lm}(\hat{\mathbf{k}})c_{\varepsilon lm\mu} .$$

Because of the spherical symmetry, the expectation value $\langle c^\dagger_{\varepsilon lm\mu}\widetilde{\mathcal{S}}c_{\varepsilon' l' m' \mu'}\rangle$ (here $\widetilde{\mathcal{S}}$ is an impurity operator) gives nonzero contribution only when $l=m=l'=m'=0$. Thus, we can replace $\psi_\mu(\mathbf{r})$ by

$$\begin{aligned}\psi_\mu(\mathbf{r})&\rightarrow\int_\varepsilon\int_{\hat{\mathbf{k}}} Y_{00}(\hat{\mathbf{k}})c_{\varepsilon 00\mu}e^{i\mathbf{k}\cdot\mathbf{r}}\\&=\int_\varepsilon\frac{\sin(k_\varepsilon r)}{k_\varepsilon r}c_{\varepsilon 00\mu} ,\end{aligned}$$

where $k_\varepsilon=|\mathbf{k}|$; we have made the energy dependence explicit. We remind the reader that $\int_\varepsilon=\int^D_{-D}\rho_0(\varepsilon)$. Since $k_\varepsilon=k_F+(\partial k/\partial\varepsilon)\varepsilon$ for the linear dispersion relation, we have $k_\varepsilon=k_F+\varepsilon/v_F$. The maximum value of $\varepsilon$ is $D$; note that $k_D r=k_F r+rD/v_F\approx k_F r$ since $rD/v_F\ll 1$. This replacement is valid, *a fortiori,* for all $\varepsilon$. Therefore, one has

$$\psi_\mu(\mathbf{r})\rightarrow\frac{\sin(k_F r)}{k_F r}\int_\varepsilon c_{\varepsilon 00\mu}=\frac{\sin(k_F r)}{k_F r}\psi_\mu(0) .$$

Using this simplification, Eq. (12) becomes

$$\begin{aligned}\widetilde{C}(r,T)=&\frac{\sin^2(k_F r)}{(k_F r)^2}\langle \psi^\dagger_\mu(0)\widetilde{\mathcal{S}}_D(\mu,\mu')\psi_{\mu'}(0)\rangle_{H_K(D)}\\&+\frac{\sin(k_F r)}{k_F r}\langle \psi^\dagger_\mu(0)\widetilde{\mathcal{S}}'_D(\mu,\mu')\psi_{\mu'}(0)+\mathrm{H.c.}\rangle_{H_K(D)}\\&+\langle \psi^\dagger_\mu(0)\widetilde{\mathcal{S}}''_D(\mu,\mu')\psi_{\mu'}(0)\rangle_{H_K(D)}+\langle \widetilde{\mathcal{U}}_D\rangle_{H_K(D)} .\end{aligned}\tag{13}$$

While the spatial dependence of the correlation function is explicit above, the temperature dependence is contained in the expectation values of the *local* operators. Thus, the calculation of the spatial and temperature dependences has been separated. The calculation of the expectation values with the renormalized Hamiltonian can be performed using a nonperturbative technique such as the Wilson renormalization-group method. Note that the restrictions on $r$ and $T$ imposed by the necessity of choosing $D$ such that $k_F r(D/D_0)\ll 1$ and $D\gg T,T_K$ have been made manifest.

The question of factorization can be investigated if we note the following. The operator $\psi^\dagger_\mu(0)$ in Eq. (13) should have been written as $\psi^\dagger_{D\mu}(0)$ to emphasize the fact $\psi^\dagger_{D\mu}(0)$ creates the most localized state that can be created at the origin with bandwidth $D$. Indeed,

$$\psi^\dagger_{D\mu}(0)=\int^D d\varepsilon\,\rho_0(\varepsilon)c^\dagger_{\varepsilon\mu} ,$$

i.e., $\psi^\dagger_{D\mu}(0)$ has reduced strength because the energy scales between $D_0$ and $D$ have been eliminated. If one defines $\widetilde{\psi}_\mu(0)$ to be the creation operator normalized to satisfy $\{\widetilde{\psi}^\dagger_\mu(0),\widetilde{\psi}_\mu(0)\}=\delta_{\mu\mu'}$, then $\psi^\dagger_\mu(0)=\sqrt{D/D_0}\,\widetilde{\psi}^\dagger_\mu(0)$. If one replaces $\psi_\mu(0)$ by the normalized operators one finds a hierarchy of contributions to $\widetilde{C}$ with powers of $\sqrt{D/D_0}$ multiplying them. Since $D/D_0\approx\frac{1}{100}$ in our calculations only the terms with no conduction-electron operators will dominate. In this example, $\widetilde{C}(r,T)$ tends to be $\langle \widetilde{U}_D\rangle_{H_K(D)}$ which is a temperature-independent function of $r$, since no impurity operators exist with nonzero expectation value in the Kondo model (except the identity operator). Thus, Eq. (13) provides important intuition about the spatial and temperature dependences of $\widetilde{C}(r,T)$. In fact, this expansion of $\widetilde{C}(r,T)$ may be viewed as an example of operator-product expansion[12] in which the expansion is dominated by the expectation values of the most localized operators (in our case, the operators which do not contain conduction-electron operators). It is easy to see that higher-order contributions to perturbative scaling preserve the general form of the expansion. This procedure will be further exemplified in the two specific contexts in Secs. III and IV. The computation of the local correlation functions in Eq. (13) also will be discussed at length.

## III. CALCULATION OF RESPONSE FUNCTION

In this section we discuss the details of the calculation of the zero-frequency response function measured in Knight-shift experiments. We also use this example to demonstrate the general recipe for calculating spatially-dependent correlation functions and zero-frequency response functions. We evaluate

$$C_1(\mathbf{r},T)=\langle\langle s_z(\mathbf{r});g_d S_z+g_e s_z\rangle\rangle_{H_K(D_0),\,\omega=0} ,\tag{14}$$

where $s_z(\mathbf{r})=\frac{1}{2}\psi^\dagger_\mu(\mathbf{r})\sigma^z_{\mu\mu'}\psi_{\mu'}(\mathbf{r})$ is the $z$ component of the conduction-electron spin density at $\mathbf{r}$ and $S_z$ is the $z$ component of the impurity spin at the origin. The Kondo Hamiltonian with cutoff $D_0$ is given by

$$H_K(D_0)=\int^{D_0}_{\varepsilon\hat{\mathbf{k}}\mu}c^\dagger_{\varepsilon\hat{\mathbf{k}}\mu}c_{\varepsilon\hat{\mathbf{k}}\mu}=\tfrac{1}{2}J_0\mathbf{S}\cdot\psi^\dagger_\mu(\mathbf{0})\boldsymbol{\sigma}_{\mu\mu'}\psi_{\mu'}(\mathbf{0}) ,\tag{15}$$

where

$$\psi_\mu^\dagger(\mathbf{r})=\int_\varepsilon^{D_0}\int_{\hat{\mathbf{k}}} c^\dagger_{\varepsilon\hat{\mathbf{k}}\mu} e^{ik_\varepsilon\hat{\mathbf{k}}\cdot\mathbf{r}} \tag{16}$$

and

$$\int_\varepsilon^{D_0}\int_{\hat{\mathbf{k}}}=\int_{-D_0}^{D_0} d\varepsilon\,\rho_0 \int d\Omega_{\hat{\mathbf{k}}}/4\pi\ . \tag{17}$$

Note that $c^\dagger_{\varepsilon\hat{\mathbf{k}}\mu}$ creates an electron with energy $\varepsilon$, wave vector along $\hat{\mathbf{k}}$, and spin $\mu$; the magnitude of the wave vector is denoted by $k_z$ where we have made the energy dependence explicit.

We generate the response function $C_1(\mathbf{r},T)$ by introducing auxiliary fields $h$ and $h_1$:

$$H_1(D_0)=H_K(D_0)-h(g_dS_z+g_es_z)-h_1s_z(\mathbf{r})\ . \tag{18}$$

$C_1$ is then obtained as a second derivative of the corresponding free energy:

$$C_1(\mathbf{r},T)=-\partial^2F_1/\partial h_1\partial h\,|_{h=h_1=0}\ , \tag{19}$$

where

$$F_1=-k_BT\ln \mathrm{Tr}e^{-\beta H_1(D_0)}\ . \tag{20}$$

The addition of terms proportional to $h$ and $h_1$ to the Hamiltonian necessitates some care in the application of perturbative scaling; we describe this in somewhat greater detail. The effect of $h$ acting on the conduction electrons (we will set $g_e=g_d=g$ in the subsequent calculations for simplicity) can be incorporated in the calculation by introducing different densities of states for the up- and down-spin electrons: $\rho_\downarrow(\varepsilon)$ which is nonzero for $\varepsilon$ in the interval $(-D_0+gh/2,D_0+gh/2)$ and $\rho_\uparrow(\varepsilon)$ which is nonvanishing in $(-D_0-gh/2,D_0-gh/2)$.

It is important at this stage to emphasize that the Hamiltonian used in the generalized scaling equations is tacitly assumed to be normal-ordered.[9] Normal ordering the Hamiltonian in Eq. (18) leads to some extra terms. The kinetic energy $\sum_\mu\int d\varepsilon\,\rho_\mu(\varepsilon)\varepsilon c^\dagger_{\varepsilon\mu}c_{\varepsilon\mu}$ yields $-\rho_0g^2h^2/2$ which does not contribute to the response function under consideration. The term $\int_{\varepsilon\mu}\int_{\varepsilon'\mu'}c^\dagger_{\varepsilon\mu}\mathcal{S}(\varepsilon\mu;\varepsilon'\mu')c_{\varepsilon'\mu'}$ contributes

$$\sum_\mu\int_0^{D_0+gh\mu} d\varepsilon\,\rho_\mu(-\varepsilon)\mathcal{S}(-\varepsilon\mu;-\varepsilon\mu)$$

which, for the Kondo interaction, gives rise to $-\rho_0J_0(gh)S_z/2$. the term proportional to $h_1$ yields $-h_1(gh)\rho_0/2$. This last term contributes $\rho_0g/2$ to $C_1$ and corresponds to the constant Knight shift due to the Pauli susceptibility; this is subtracted out in the expression for $\Delta K$ [see Eq. (3)].

Having normal ordered the Hamiltonian carefully, we can use the generalized recursion relations to integrate out the up-spin hole degrees of freedom with energies between $-D_0-gh/2$ and $-D_0+gh/2$ and down-spin electron degrees of freedom with energies between $D_0+gh/2$ and $D_0-gh/2$ to obtain a symmetric, spin-independent density of states. This yields contributions to both $\mathcal{U}$ and $\mathcal{S}$ to order $O((\rho_0J_0)^2)$. For example, $\delta\mathcal{U}$ contains a term $gh(\ln 2)(\rho_0J_0)^2(\frac{3}{4}-S_z)/2$ that only leads to $O((\rho_0J_0)^3)$ corrections (in overall multiplicative factor) to $C_1(r,T)$. Since we will focus on determining the $r$ dependence of $C_1$ to $O(\rho J)$, we can ignore these contributions. Thus, we reduce the Hamiltonian to

$$H_1(D_0)=H_K(D_0)-hgS_z-h_1s_z(\mathbf{r})-h_1h(g\rho_0/2)\ . \tag{21}$$

The term of the form $\rho_0J_0ghS_z/2$ is also ignored because we are only interested in determining the $r$ dependence of $C_1$ to $O(\rho J)$.

Since thermodynamic scaling theory preserves the free energy [up to terms of $O(e^{-D/k_BT})$], we can use the effective Hamiltonian at the reduced bandwidth $D$ to calculate $C_1$ instead of $H_1(D_0)$. We have retained terms up to $O(h)$, $O(h_1)$, and $O(h,h_1)$ in applying perturbative scaling formalism, since these are sufficient to evaluate $C_1$ [see Eqs. (18)–(20)]. We use $H_1(D_0)$ as the initial Hamiltonian and apply the recursion relations to second order. We find that several new terms proportional to $h$, $h_1$, or $hh_1$ are generated. The general form of the effective Hamiltonian $H(D)$ is given by

$$\begin{aligned}H(D)=&\int_\varepsilon^D\int_{\hat{\mathbf{k}}\mu}\varepsilon c^\dagger_{\varepsilon\hat{\mathbf{k}}\mu}c_{\varepsilon\hat{\mathbf{k}}\mu}-\tfrac{1}{2}J(D)\mathbf{S}\cdot\psi^\dagger(0)\boldsymbol{\sigma}\psi(0)+E_0+\left[\frac{-\rho_0g_e}{2}+E_1\right]hh_1+S_z[U_0h+U_1(\mathbf{r},D)h_1+U_2(\mathbf{r},D)hh_1]\\&+h_1\{K_1(\mathbf{r},D)S_z\psi^\dagger(0)\psi(0)-\tfrac{1}{2}J_1(r,D)\psi^\dagger(0)\sigma_z\psi(0)-\tfrac{1}{2}K_t(\mathbf{r},D)S_z[\psi^\dagger(\mathbf{r})\psi(0)+\psi^\dagger(0)\psi(\mathbf{r})]\\&-\tfrac{1}{2}J_x(r,D)i\varepsilon^{mn3}S_m[\psi^\dagger(\mathbf{r})\sigma_n\psi(0)-\psi^\dagger(0)\sigma_n\psi(\mathbf{r})]-\tfrac{1}{2}\psi^\dagger(\mathbf{r})\sigma_z\psi(\mathbf{r})\}\ .\end{aligned} \tag{22}$$

A brief note on notation: $E_0$ and $E_1$ refer to ground-state energies. Terms that involve only impurity operators $(S_z)$ have coefficients $U_0$, $U_1$, and $U_2$. Couplings denoted by $K$ involve (impurity-spin-independent) potential scattering of conduction electrons while $J$'s refer to scattering which depends on conduction-electron spins. The subscript $t$ indicates a transfer of a conduction electron from 0 to $\mathbf{r}$ vice versa and the subscript $x$ refers to the cross-product nature of the interaction. We have explicitly separated out the dependence on $h$, $h_1$, and $hh_1$. Except for the constant terms and $J$, which has dimensions of energy, all other couplings $(U_0,U_1,U_2,K_1,\ldots)$ are dimensionless.

The recursion relations can be derived by straightforward, tedious algebra using Eqs. (9) and (10). In the notation of the generalized impurity Hamiltonian in Eq. (8), the operators $\mathcal{S}$ and $\mathcal{U}$ are given by

$$\mathcal{U}_D=E_0+(-\rho_0g/2+E_1)hh_1+S_z(-h-U_1h_1-U_2hh_1) \tag{23}$$

and

$$\mathcal{S}_D(\varepsilon\zeta\mu;\varepsilon'\zeta'\mu')=-\frac{J(D)}{2}\mathbf{S}\cdot\boldsymbol{\sigma}_{\mu\mu'}+K_1(D)h_1S^z\delta_{\mu\mu'}$$
$$-\tfrac{1}{2}h_1[J_1(D)\sigma^z_{\mu\mu'}+K_tS^z\delta_{\mu\mu'}(e^{ik\zeta r}+e^{-k'\zeta' r})+iJ_x\varepsilon^{3lm}S^l\sigma^m_{\mu\mu'}(e^{ik\zeta r}-e^{-ik'\zeta' r})+e^{i(k\zeta-k'\zeta')r}\sigma_{\mu\mu'}]\ , \qquad (24)$$

where $\zeta$ denotes $\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}$ and $\zeta'$ denotes $\hat{\mathbf{k}}'\cdot\hat{\mathbf{r}}'$ Substituting Eqs. (23) and (24) to Eqs. (9) and (10) and performing spin sums and angular integrals which lead to the $r$ dependence of the coupling constants, we obtain the recursion relations. The reader interested in the details of the algebraic drudgery involved in the derivation of such recursion relations may write to the authors. The coupling constants evolve according to the following differential equations:

$$-D\frac{dJ}{dD}=-\rho_0J^2\ , \qquad (25)$$

$$-D\frac{dK_t}{dD}=-\rho_0JJ_x+\frac{\rho_0J}{2}(\phi_D-\phi_{-D})\ , \qquad (26)$$

$$-D\frac{dJ_x}{dD}=-\tfrac{1}{2}\rho_0(JJ_x+JK_t)+\tfrac{1}{2}\rho_0J(\phi_D-\phi_{-D})\ , \qquad (27)$$

$$-D\frac{dJ_1}{dD}=-\tfrac{1}{2}\rho_0(\phi_D-\phi_{-D})(JJ_x-\tfrac{1}{2}JK_t)\ , \qquad (28)$$

$$-D\frac{dK_1}{dD}=-\tfrac{1}{2}\rho_0(\phi_D+\phi_{-D})JJ_x\ , \qquad (29)$$

$$\frac{dU_1}{dD}=-\rho_0^2\int_0^D\frac{d\varepsilon}{D+\varepsilon}[2J_1J+JJ_x(\phi_D+\phi_\varepsilon-\phi_{-D}-\phi_{-\varepsilon})$$
$$+J(\phi_D\phi_{-\varepsilon}+\phi_{-D}\phi_\varepsilon)]\ . \qquad (30)$$

As in the earlier section, we have $\phi_D=\sin(k_Dr)/k_Dr$, $\phi_\varepsilon=\sin(k_\varepsilon r)/k_\varepsilon r$, and $k_\varepsilon=k_F+\varepsilon/v_F$. Note that it is through the functions $\phi_D$ and $\phi_\varepsilon$ that the coupling constants develop $r$ dependence. We have not displayed the recursion relation for $E_1$, because its explicit form will not be needed; it is complicated and its order of magnitude is estimated later in this section.

### A. Response function within scaling theory

Consider integrating the second-order recursion relations from an initial bandwidth of $D_0$ down to $D$ where the conditions described in the previous section, i.e., $k_Fr \ll D_0/D$ and $T,T_K \ll D$ are satisfied. This is, as emphasized earlier, within the range of validity of the perturbative scaling equations. None of the couplings has grown large, but the separation of spatial and thermal dependences is nevertheless possible. As described in Sec. II we can keep only $s$-wave conduction-electron operators because of the spherical symmetry of the original Hamiltonian; this leads to

$$C_1(r,T)=\rho_0g/2+E_1+U_1\langle\langle S_z;S_z\rangle\rangle_{H_K(D)}+\left[-K_1+K_t\frac{\sin(k_Fr)}{k_Fr}\right]\frac{D}{D_0}\langle\langle S_z;S_z\tilde{\Psi}^\dagger_\mu(0)\tilde{\Psi}_\mu(0)\rangle\rangle_{H_K(D)}$$
$$+\left[J_1+\left[\frac{\sin(k_Fr)}{k_Fr}\right]^2\right]\frac{D}{D_0}\langle\langle S_z;\tilde{\Psi}^\dagger_\mu(0)(\tfrac{1}{2}\sigma^z_{\mu\mu'})\tilde{\Psi}_{\mu'}(0)\rangle\rangle_{H_K(D)}\ , \qquad (31)$$

where $\tilde{\Psi}$, defined by

$$\Psi(0)=\sqrt{D/D_0}\tilde{\Psi}(0)\ ,$$

obeys the canonical commutation relations. Observe that the running coupling constants $U_1$, $K_1$, $K_t$, $J_1$, etc., themselves have $r$ dependence, obtained from integrating the recursion relations Eqs. (25)–(30). It is important to emphasize that no singularities occur in the transformation relating $C_1(r,T)$ to the local response functions; in particular, there are no singularities in the $r$ dependent coefficients. Thus, this expression is valid for $T<T_K$ as well. The logarithmic divergences that plague the perturbative calculation of the response functions and correlation functions (see, for example, Ref. 13) are now buried in the local response functions which, therefore, have to be calculated nonperturbatively.

The expression for $dU_1/dD$ [in Eq. (30)] is only accurate to first order in $J$ because the energy dependences that are generated in second order have not been included. We have identified all the second-order contributions to $dU_1/dD$; they can be calculated if greater quantitative accuracy is necessary, but this involves considerable tedium. Howerer, the first-order result is sufficient to deduce the generic features of $C_1(r,T)$ and demonstrate the remarkable accurate factorization of spatial and thermal dependences. Higher-order corrections will only modify the spatial dependence but will not affect the factorization. We have estimated and shown in this particular case that the second-order contribution is *small.*

Now consider the various terms on the right-hand side of Eq. (31). We remind the readers that all opeartors that appear in the Hamiltonian and in the response or correlation functions are in normal-ordered form. Because the original Hamiltonian is particle-hole symmetric, $\langle\langle S_z;S_z\tilde{\Psi}^\dagger(0)\tilde{\Psi}(0)\rangle\rangle_{H_K(D)}$ is zero. Even if the Hamiltonian is not particle-hole symmetric, the contribution due to this term is down by a factor of $D/D_0$. We will comment on the effects of the violation of particle-hole symmetry later.

We will now argue that the contribution due to the constant term $E_1$ in Eq. (31) can be ignored. To do this we estimate the order of magnitude of $E_1$. The dependence on the field $h$ in the term $-E_1 h h_1$ comes from the corresponding $h$ dependence in the energy denominator

$$1/(D \pm h/2) = (1/D) \mp (h/2)(1/D^2) .$$

As a result, the recursion relation for $E_1$ has an additional factor of $1/D$ compared to that for $U_1(r,D)$. Consequently, after integrating the recursion relations, $E_1$ is of the order of

$$\rho_0 \ln(D_0/D)(\rho_0 J_0)^2 \approx (1/D_0)\ln(D_0/D)(\rho_0 J_0)^2 ,$$

compared to the term $U_1(r,D)\langle\langle S_z;S_z\rangle\rangle$ which is of the order of $\rho_0 J_0[1/\max(T,T_K)]$ (see next section for this estimate). $E_1$ is down by roughly a factor of $\rho_0 J_0 \max(T,T_K)\ln(D_0/D)/D_0$, and is negligible. [For a typical Kondo system, Fe in Cu, one has $T_K/D_0 = (1-5)\times 10^{-4}$, $\rho_0 J_0 = -(0.1-0.2)$; with $D/D_0 \sim 0.01$ this factor is of order $10^{-3}$.] Thus, only two terms remain:

$$C_1(r,T) = U_1 \langle\langle S_z;S_z\rangle\rangle_{H_K(D)} + \frac{1}{2}\left[J_1 + \left(\frac{\sin(k_F r)}{k_F r}\right)^2\right]\frac{D}{D_0} \times \langle\langle S_z;\tilde{\Psi}^\dagger_\mu(0)\sigma^z_{\mu\mu'}\tilde{\Psi}_{\mu'}(0)\rangle\rangle_{H_K(D)} . \tag{32}$$

Here, we have redefined $C_1(r,T)$ as $C_1(r,T) - \rho_0 g/2$, which is proportional to $\Delta K(r,T)$ with the constant Knight shift due to the conduction electrons being subtracted out [see Eq. (3).]

### B. Factorization of the spatial and temperature dependences

It was argued in the previous section that the terms associated with local response (or condition) functions involving conduction-electron operators can be neglected. We verify the argument in the context of $C_1(r,T)$ by estimating the magnitude of two terms in the rhs of Eq. (32) explicitly. We will show that the second term is indeed down by a factor of $D/D_0$ and can be neglected; hence, we have

$$C_1(r,T) = U_1 \langle\langle S_z;S_z\rangle\rangle_{H_K(D)} . \tag{33}$$

We outline the argument below: The first term, $U_1(r)$, can be estimated from the recursion relations and is of the order of $\rho_0 J_0$. It is clear that $\langle\langle S_z;S_z\rangle\rangle_{H_K(D)}$ is essentially the same as the response function $\langle\langle S_z;S_z\rangle\rangle_{H_K(D_0)}$ calculated with the original Hamiltonian at cut off $D_0$ for $T \ll D$. More explicitly, $\langle\langle S_z;S_z\rangle\rangle_{H_K(D_0)}$ is proportional to the impurity susceptibility which, in turn, has the form $f(T/T_K)/T$, where $f(T/T_K)$ is a universal function [$T_k$ for $H_K(D_0)$ and that for $H_K(D)$ are slightly different due to the neglect of the higher-order terms in perturbative scaling]. Thus, $\langle\langle S_z;S_z\rangle\rangle_{H_K(D)}$ is essentially the impurity susceptibility and is of order of $[1/\max(T,T_k)]$. Consequently, the first term is of order of $\rho_0 J_0[1/\max(T,T_K)]$ for small $r$.

Now consider the second term. The coefficient is of the order of $D/D_0$, and, hence, if the response function can be assumed to remain bounded as the temperature is lowered then it can be neglected. We have calculated the response function $\langle\langle S_z;\tilde{\Psi}^\dagger_\mu(0)(\frac{1}{2}\sigma^z_{\mu\mu'})\tilde{\Psi}_{\mu'}(0)\rangle\rangle_{H_K(D)}$ using Wilson's *nonperturbative,* numerical RG method. We will show below that this response function is proportional to $\langle\langle S_z;S_z\rangle\rangle$ and is of the order of

$$\rho_0 J_0 \langle\langle S_z;S_z\rangle\rangle \approx \rho_0 J_0[1/\max(T,T_K)] .$$

Thus, the second term is indeed a factor of $D/D_0$ smaller. This immediately implies factorization [Eq. (33)]; the form of the spatial dependence will be evaluated later. The thermal dependence is obviously proportional to the susceptibility.

### C. The Wilson RG method

We introduce some of the relevant notation used in Wilson's *nonperturbative* renormalization-group approach (the reader may consult Refs. 10, 14, and 15 for details) and present an outline of the extensions required to compute local, zero-frequency response functions and correlation functions, some of the details being relegated to the Appendices.

#### *1. Discretization*

Consider the Kondo Hamiltonian $H_K$. It is convenient to measure energies in units of the bandwidth $D_0$. The energy interval from $-1$ to 1 is then discretized *logarithmically:* the $n$th interval for positive $\varepsilon$ extends from $\Lambda^{-n-1}$ to $\Lambda^{-n}$, where $\Lambda > 1$. Wilson then replaces the continuous set of energy levels in each interval by single levels and rewrites the Hamiltonian in terms of operators that create these discrete levels. A further tridiagonalization leads to the following form for the Hamiltonian:

$$H = \frac{1+\Lambda^{-1}}{2}\left[\sum_{n=0}^{\infty}\Lambda^{-n/2}\xi_n(f^\dagger_{n\mu}f_{n+1\mu} + f^\dagger_{n+1\mu}f_{n\mu}) - \tilde{J} f^\dagger_{0\mu}\tfrac{1}{2}\boldsymbol{\sigma}_{\mu,\mu'}f_{0\mu'}\cdot\mathbf{S}\right] , \tag{34}$$

where $\tilde{J} = 4(1+\Lambda^{-1})^{-1}\rho_0 J_0$ and $\xi_n$ is given by

$$\xi_n = (1-\Lambda^{-n-1})(1-\Lambda^{-2n-1})^{1/2}(1-\Lambda^{-2n-3})^{1/2} \tag{35}$$

whose value rapidly approaches unity for large $n$. We recall the physical interpretation of the new basis. The $\{f^\dagger_{n\mu}\}$ create electron states with mean energy zero (i.e., at the Fermi level) with a spread in energy $\Lambda^{-n/2}$; the states have a spatial extent $\Lambda^{n/2}$ (in units of $k_F^{-1}$) around the impurity. Note that the impurity spin only couples to the state created by $f^\dagger_0$, while the state created by $f^\dagger_n$ only couples to those created by $f^\dagger_{n+1}$ and $f^\dagger_{n-1}$.

In order to solve the Hamiltonian in Eq. (34), we define a sequence of Hamiltonians $H_N$ where $\{H_N\}$ is obtained from $H$ defined in Eq. (34) by truncating the upper limit of the summation at $n=N$ and multiplying by a rescaling factor

$$R_N = \frac{2}{1+\Lambda^{-1}} \Lambda^{(N-1)/2} .$$

It is easy to see that the sequence $\{H_N\}$ satisfies the following recursion relation:

$$H_{N+1} = \Lambda^{1/2} H_N + H_{NI} ,$$

where

$$H_{NI} = \xi_N (f^\dagger_{N\mu} f_{N+1,\mu} + f^\dagger_{N+1,\mu} f_{N\mu}) \text{ for } N \geq 1 .$$

This recursion relation defines the *renormalization-group transformation.* Beginning with $H_0$, which contains the coupling to the impurity spin, we can successively generate and diagonalize $H_1$, $H_2, \ldots$ . The RG structure is determined by the way the low-energy levels (which determine the low-temperature behavior) evolve.[16] The truncation of the high-energy states can be performed at each step without affecting the low-energy levels, and this is the essence of the RG transformation.

Now we recall the basic scheme of the recursive procedure: Let $|l,N\rangle$ denote the eigenstates of $H_N$, where $l = 0, \ldots, L_N$ ($l = 0$ represents the ground state of $H_N$). $L_N$ will be given by $2^{(2N+3)}$ if we retain all the states. The Hamiltonian $H_{N+1}$ can be diagonalized in a basis generated from the eigenstates of $H_N$ using the operators $f^\dagger_{N+1\mu}$. Thus, the eigenstates $|l,N+1\rangle$ of $H_{N+1}$ and their energies $E(l,N+1)$ are determined. Now one is ready to solve for $H_{N+2}$, and so on.

In order to make this procedure numerically feasible, we truncate the matrices so that only low-energy states (energy smaller than 10, for example) are retained and we exploit various symmetries of the Hamiltonian. Since the total charge and spin are conserved, every eigenstate of $H_N$ can be classified according to its value of $Q$, $S^2$, and $m_S$ (the $z$ component of the total spin) at the $N$th stage of the iteration:

$$\begin{aligned} Q_N &= \sum_{n=0}^{N} (f^\dagger_{n\mu} f_{n\mu} - 1) , \\ \mathbf{S}_N &= \tfrac{1}{2} \sum_{n=0}^{N} f^\dagger_{n\mu} \boldsymbol{\sigma}_{\mu\nu} f_{n\mu} + \mathbf{S}_{\text{imp}} . \end{aligned} \tag{36}$$

One can avoid having to keep track of $m_S$ by using Clebsch-Gordan coefficients and working entirely in terms of the reduced matrix elements $\langle Q,S \| f^\dagger_N \| Q',S' \rangle$. The energy eigenvalues will be independent of $m_S$.

For the details of this procedure, see Appendix B in the paper by Krishnamurthy *et al.*[14] The corresponding details for the case when $S^2$ is not conserved are given in Appendix B of the present paper.

### 2. *Thermodynamic quantities*

We use calculation of the impurity susceptibility as an example to illustrate the formalism for calculating thermodynamic quantities. The susceptibility is defined by

$$T\chi_{\text{imp}}(T) = \frac{\text{Tr}[S_z^2 \exp(-\beta H_K)]}{\text{Tr}\exp(-\beta H_K)} - \frac{\text{Tr}[S_{0z}^2 \exp(-\beta H_c)]}{\text{Tr}\exp(-\beta H_c)} , \tag{37}$$

where $S_z$ is the $z$ component of the total spin and $S_{0z}$ is the $z$ component of the conduction-electron spin. The original Hamiltonian $H_K$ is recovered by

$$H_K = \lim_{M\to\infty} \left[ D\Lambda^{-(M-1)/2} \left[ \frac{1+\Lambda^{-1}}{2} \right] H_M \right\} . \tag{38}$$

Crudely speaking, information about the many-particle energy-level structure of $H_K$ at energies $[2/(1+\Lambda^{-1})]\Lambda^{-(N-1)/2}D$ is contained in the level structure of $H_N$ at an energy scale of 1. This motivates the definition of an inverse temperature

$$\bar{\beta}_M = \beta[\tfrac{1}{2}(1+\Lambda^{-1})] D_0 \Lambda^{-(M-1)/2} .$$

Obviously, one cannot calculate expectation values in the limit $M \to \infty$ directly. We can only evaluate the expression at finite values of $N$. Consider the problem of evaluating $\chi(T)$ at a low temperature $T$ to a chosen accuracy. Given a $\Lambda$, we choose an appropriate small $\bar{\beta}$ and an $N$ such that $\bar{\beta}_N = \bar{\beta}$. Consider $M > N$. We split $H_N$ from $H_M$ and the operators $\mathbf{S}_N$ from $\mathbf{S}_M$ by separating the set of operators $\{\mathbf{S}, f_0, \ldots, f_N\}$ from $\{f_{N+1}, \ldots, f_M\}$. The part of the Hamiltonian that couples $H_N$ to $H_M$ is treated as a perturbation $H_I$. At zeroth order in $H_I$, the susceptibility is given by

$$T_N \chi(T_N) \approx \frac{\text{Tr}[S_{Nz}^2 \exp(-\bar{\beta} H_N)]}{\text{Tr}\exp(-\bar{\beta} H_N)} - \frac{\text{Tr}[S_{0Nz}^2 \exp(-\bar{\beta} H_{0N})]}{\text{Tr}\exp(-\bar{\beta} H_{0N})} . \tag{39}$$

This can be evaluated quite accurately, if we keep all energy levels with $\bar{\beta} E_N \leq 10$. The perturbation correction to first order in $H_I$ can be shown to vanish. The second-order contribution involves matrix elements of $f_N$, which are calculated and stored at each stage of the RG procedure. The details are contained in Appendix B of Ref. 14. Thus, we can compute $\chi$ at a sequence of temperatures determined by $\bar{\beta}_N = \bar{\beta}$,

$$T_N = D \frac{1+\Lambda^{-1}}{2} \Lambda^{-(N-1)/2} / \bar{\beta} ,$$

to an accuracy of $\bar{\beta}/\Lambda$. $N$ defines a logarithmic temperature scale.

In practice, one cannot choose $\bar{\beta}$ to be very small since we must keep all energy levels up to an energy of roughly about $10/\bar{\beta}$ to avoid large truncation errors. On the other hand, large $\bar{\beta}$ makes the inclusion of $H_I$ to second order in perturbation theory insufficient. The compromise adopted in practice is to choose $\bar{\beta}$ to be around and smaller than 1.

### 3. *Calculation of local response functions and correlation functions*

We have generalized the approach outlined above to the calculation of local correlation functions and zero-frequency response functions. The additional complication arises from the need to keep track of the matrix elements of operators: Consider the calculation of the correlation function $\langle \hat{A} \rangle$. At the $N$th iteration we have to keep track of the matrix elements of $\hat{A}$, $\langle Q,S \| \hat{A} \| Q',S' \rangle$, in addition to the matrix elements $\langle Q,S \| f_N^{\dagger} \| Q',S' \rangle$ and the eigenenergies $E(Q,S)$.

Following the earlier discussion, we split the operator $\hat{A}$

$$\hat{A}_M = \hat{A}_N + \hat{A}_{M,N+1} ,$$

where $\hat{A}_N$ is the part containing the operators $\{f_0, \ldots, f_N\}$ and $\hat{A}_{N+1,M}$ is the part containing the operators $\{f_{N+1}, \ldots, f_M\}$. For the local correlation functions we have considered, $\hat{A}_{N+1,M}=0$.

We can write $\langle \hat{A} \rangle$ to zeroth order in $H_{NI}$ as

$$\langle \hat{A} \rangle = \frac{\operatorname{Tr}(\hat{A} e^{-\bar{\beta} H_N})}{\operatorname{Tr} e^{-\bar{\beta} H_N}} = \frac{\sum_{Q,S,r} \langle Q,S,r | \hat{A} | Q,S,r \rangle e^{-\bar{\beta} E_N(Q,S,r)}}{\sum_{Q,S,r} e^{-\bar{\beta} E_N(Q,S,r)}} . \tag{40}$$

The contribution to first order in $H_{NI}$ vanishes while the second-order correction is quite complicated, particularly when $\hat{A}$ does not commute with $H_N$. It is presented in Appendix A.

The calculation of local zero-frequency response functions is more complicated since the total spin $S$ is no longer conserved in the cases of interest. We need to change some of the details of the original procedure of Wilson. To illustrate the basic idea, we discuss the calculation of $\tilde{\chi}$ which is the impurity susceptibility of the Kondo Hamiltonian, if the conduction-electron $g$ factor is set equal to zero: $\tilde{\chi} = \langle\langle S_z ; S_z \rangle\rangle$, where $S_z$ is the $z$ component of the impurity spin. We have seen that the impurity susceptibility can also be defined as $T\chi = \langle S_{tz}^2 \rangle_{H_K} - \langle S_{tz}^2 \rangle_{H_c}$, where $S_{tz}$ is the total spin of the system, and $H_c$ is the conduction-electron Hamiltonian only. This is the expression Wilson used to calculate the impurity susceptibility.

We start with the expression

$$\langle\langle S_z ; S_z \rangle\rangle = (\partial \langle S_z \rangle_H / \partial h)_{h=0} = \lim_{h \to 0} \frac{\langle S_z \rangle_H}{\beta h}$$

where $H = H_K - h S_z$. When $h \ll T, T_K$, the expectation value $\langle S_z \rangle_H$ is linear in $h$. We have verified this explicitly in our numerical calculations.

The presence of the term $hS_z$ in the Hamiltonian implies that the total spin $S$ is no longer conserved and, hence, we can only diagonalize the Hamiltonian in $(Q, m_S)$ subspace. As a consequence, one has to diagonalize larger matrices than before. The details of the recursive procedure and the expressions for the second-order contribution to the response functions are given in Appendix B.

A notable numerical fact is that the second-order contribution to the susceptibility $\tilde{\chi} (= \langle\langle S_z ; S_z \rangle\rangle)$ is very small, smaller than 1% for $\bar{\beta}$ as large as 1.5 (although the second-order contribution to the partition function is not small). In contrast, the second-order contribution cannot be neglected in the procedure used by Wilson, particularly at low temperatures, even for $\bar{\beta}$ as small as 0.5. A probable reason for this fortuitous occurrence is that the conduction-electron states $\{f_{n\mu}\}$ for $n > N$ do not contribute directly to $\langle S_z \rangle_H$ while they do to the total spin $m_S$ of the many-body states in Wilson's calculation.

Because $\bar{\beta}$ can be taken as large as 1.5, we can keep fewer energy states. Typically, we retained 150–270 states; $\bar{\beta}$ was taken to be 1.501, 1.308, 1.140, 0.994, and 0.867. The calculation was done for $\Lambda=3$ and $h=10^{-3} T_K$.

In order to check the validity of this method numerically, we have compared the susceptibility calculated by this method with that obtained from Wilson's original method and found that the differences are less than 2% for the temperature range $T/T_K = 1.0 \times 10^{+4}$ to $1.0 \times 10^{-2}$ (the calculation was done for $\rho_0 J_0 = -0.1$ and $\bar{\beta}=0.866$). In making the comparison, we relate $\chi$ to $\tilde{\chi}$ by

$$\chi = [1 + \rho_0 J_0 + O((\rho_0 J_0)^2)] \tilde{\chi} . \tag{41}$$

This can be shown easily as follows: Recall that $\chi$ is defined as

$$\begin{aligned} \chi &= \langle\langle S_z + s_z ; S_z + s_z \rangle\rangle_{H_K} - \langle\langle s_z ; s_z \rangle\rangle_{H_c} \\ &= \langle\langle S_z ; S_z \rangle_{H_K} + 2 \langle\langle S_z ; s_z \rangle\rangle_{H_K} \\ &\quad + (\langle\langle s_z ; s_z \rangle\rangle_{H_K} - \langle\langle s_z ; s_z \rangle\rangle_{H_c}) . \end{aligned} \tag{42}$$

Here $s_z$ refers to the $z$ component of the total conduction-electron spin. The second term on the rhs of Eq. (42) can be written as

$$\langle\langle S_z ; s_z \rangle\rangle = -\frac{\partial}{\partial h} \frac{\partial}{\partial h_1} \ln \operatorname{Tr} e^{-\beta H_1} \tag{43}$$

with $H_1 = H_K - h_1 S_z - h s_z$. As in the case for calculating $C_1(r,T)$ [see the discussion which leads to Eq. (21)], we normal order the Hamiltonian $H_1$, integrate out the up-spin hole and down-spin electron degrees of freedom with energies between $D_0 + gh/2$ and $D_0 - gh/2$ and obtain

$$H_1 = H_K - h_1 S_z - [\tfrac{1}{2} \rho_0 J_0 + O((\rho_0 J_0)^2)] h S_z . \tag{44}$$

This immediately leads to

$$\langle\langle S_z ; s_z \rangle\rangle = [\tfrac{1}{2} \rho_0 J_0 + O((\rho_0 J_0)^2)] \langle\langle S_z ; S_z \rangle\rangle .$$

By the same method we can show that

$$\langle\langle s_z ; s_z \rangle\rangle = O((\rho_0 J_0)^2) \langle\langle S_z ; S_z \rangle\rangle .$$

Substituting these results into Eq. (42), we obtain Eq. (41). At very low temperatures, we believe that this new procedure for calculating $\chi$ is more reliable because of the smaller second-order contribution to $\tilde{\chi}$.

### D. Results of calculation

Numerical calculations were done for $\rho_0 J_0 = -0.075$, $-0.10$, and $-0.15$. The corresponding Kondo temperatures determined by

$$T_K = D_0\sqrt{|\rho_0 J_0|}\,e^{-1/|\rho_0 J_0|}$$

are $T_K/D_0 = 4.11\times10^{-7}$, $1.44\times10^{-5}$, and $4.93\times10^{-4}$, respectively. At the reduced cutoff $D = 10^{-2}D_0$, the corresponding values of $\rho_0 J(D)$ calculated from second-order scaling are $\rho_0 J(D) = -0.114$, $-0.185$, and $-0.485$.

We have calculated the response function $\langle\langle S_z;\sigma_z(0)\rangle\rangle$ with both $H_K(D_0)$ and $H_K(D)$, where $\sigma_z(0) = \tilde{\Psi}^{\dagger}_{\mu}(0)(\frac{1}{2}\sigma^z_{\mu\mu'})\tilde{\Psi}_{\mu'}(0)$ is the conduction-electron spin density at the origin. In all cases,

$$\langle\langle S_z;\sigma_z(0)\rangle\rangle_{H_K(\bar{D})}/\langle\langle S_z;S_z\rangle\rangle_{H_K(\bar{D})}$$

(where $\bar{D} = D_0$ or $D$) is constant (variation with temperature smaller than 1%) for $T \le \bar{D}/10$. Therefore, at low temperatures,

$$\langle\langle S_z;\sigma_z(0)\rangle\rangle_{H_K(\bar{D})} = g[\rho_0 J(\bar{D})]\langle\langle S_z;S_z\rangle\rangle_{H_K(\bar{D})}\ . \tag{45}$$

The values of $g[\rho_0 J(\bar{D})]$ for two sets of values of the coupling constants $J(\bar{D})$ (one set consists of values of the initial coupling with cutoff $D_0$ and the other set of the values of the corresponding couplings with cutoff $D$ obtained from perturbative scaling) are given in Table I. For comparison, we also list in the table the results from perturbative scaling: Substituting $r=0$ in our result for $\langle\langle S_z;\sigma_z(r)\rangle\rangle$ in Eq. (32), we have

$$\langle\langle S_z;\sigma_z(0)\rangle\rangle = U_1(0)\langle\langle S_z;S_z\rangle\rangle\ .$$

$U_1(0)$ can be calculated from the recursion relations [Eqs. (25)–(30)] and is listed in the table. We see that perturbative scaling theory yields qualitatively correct results, i.e., $\langle\langle S_z;\sigma_z(0)\rangle\rangle$ is proportional to $\langle\langle S_z;S_z\rangle\rangle$ at low temperatures ($T \ll D$). The proportionality constant is also quantitatively reasonable to first order in $J$ (the difference between $g$ and $U_1$ is within 10% for $\rho J \approx 0.1$). From our nonperturbative numerical results we found that

$$g(\rho_0 J(\bar{D})) = g_0\rho_0 J(\bar{D}) + g_1[\rho_0 J(\bar{D})]^2 \tag{46}$$

with $g_0 \approx 0.65$ and $g_1 \approx -0.7$.

In our numerical calculations, we have used $\Lambda = 3$. Because $g(\rho_0 J(\bar{D}))$ is not an universal quantity, we expect it to display stronger dependence on $\Lambda$ than in the case of universal quantities. We have performed calculations for $\Lambda = 2.1615$ and 3.948 to check the $\Lambda$ dependence of $g$. For $\rho_0 J_0 = -0.1$, $g(\rho_0 J(\bar{D})) = -0.0695$ when calculated with $\Lambda = 3.948$ and $g(\rho_0 J(\bar{D})) = -0.0727$ when calculated with $\Lambda = 2.616$ [remember that $g(\rho_0 J(\bar{D})) = -0.0718$ when calculated with $\Lambda = 3$]. We can see some variation (smaller than 5%) in the range $\Lambda = 2.6$–4.0. However, the fact that $\langle\langle S_z;\sigma_z(0)\rangle\rangle$ is proportional to $\langle\langle S_z;S_z\rangle\rangle$ for $T < \bar{D}/10$ holds very accurately for all the $\Lambda$'s. This proportionality is another example of the operator-product expansion alluded to in the Introduction. For completeness we have displayed $\langle\langle S_z;\sigma_z(0)\rangle\rangle/\langle\langle S_z;S_z\rangle\rangle$ as a function of temperature in Fig. 1.

The proportionality of $\langle\langle S_z;\sigma_z(0)\rangle\rangle$ to $\langle\langle S_z;S_z\rangle\rangle$ with a coefficient $\rho J$ to leading order justifies the neglect of the second term in Eq. (32), which is down by an additional

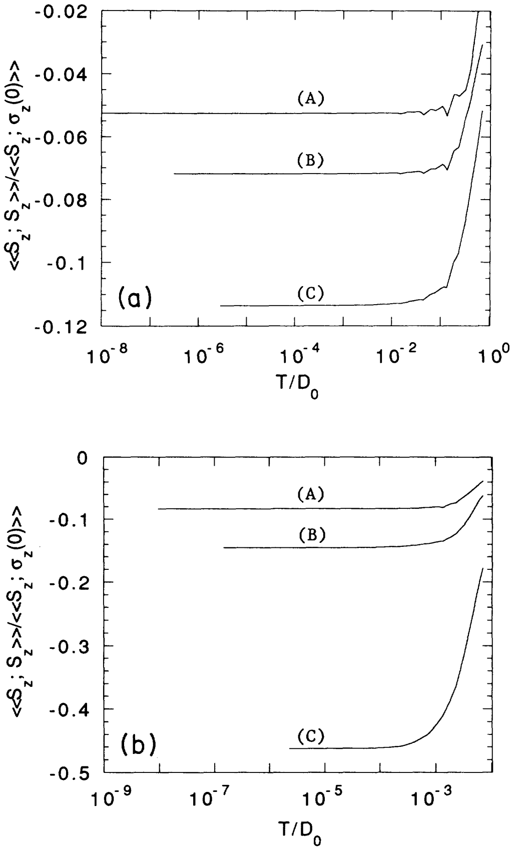

FIG. 1. (a) The ratio of two response functions $\langle\langle S_z;\sigma_z(0)\rangle\rangle_{H_K(\bar{D})}/\langle\langle S_z;S_z\rangle\rangle_{H_K(\bar{D})}$ as a function of temperature (in units of $D_0$) for $\rho_0 J(\bar{D}) =$ (A) $-0.075$, (B) $-0.10$, (C) $-0.15$ at $\bar{D} = D_0$. (b) The ratio of two response functions $\langle\langle S_z;\sigma_z(0)\rangle\rangle_{H_K(\bar{D})}/\langle\langle S_z;S_z\rangle\rangle_{H_K(\bar{D})}$ as a function of temperature (in units of $D_0$) for the corresponding renormalized coupling at $\bar{D} = D = D_0/100$ for $\rho_0 J(\bar{D}) =$ (A) $-0.114$, (B) $-0.185$, (C) $-0.485$.

TABLE I. Ratios $g/\rho_0 J(\bar{D})$ at low temperatures for two sets of couplings at $\bar{D} = D_0$ and $\bar{D} = D$, respectively. The corresponding ratios $U_0$ from perturbative scaling are also listed for comparison.

| | Bandwidth $D_0$ | | | Bandwidth $D$ | | |
|---|---|---|---|---|---|---|
| $\rho_0 J(\bar{D})$ | $-0.075$ | $-0.10$ | $-0.15$ | $-0.114$ | $-0.185$ | $-0.485$ |
| $g$ | $-0.0525$ | $-0.0718$ | $-0.114$ | $-0.0830$ | $-0.145$ | $-0.462$ |
| $g/\rho_0 J(\bar{D})$ | 0.700 | 0.718 | 0.760 | 0.728 | 0.784 | 0.952 |
| $U_1(0)$ | $-0.0557$ | $-0.0767$ | $-0.124$ | | | |

factor of $D/D_0$. We have thus given a first-principles proof of the factorization of the $r$ and $T$ dependences of the response function which describes the extra NMR Knight shift. The remaining term is proportional to $\tilde{\chi}=\langle\langle S_z;S_z\rangle\rangle$ with a coefficient $U_1(r)$ that is discussed below. The temperature dependence arises from the zero-frequency response function. As we have seen to leading order in perturbation theory, $\tilde{\chi}=(1-\rho_0 J_0)\chi$.

In Fig. 2, we have plotted the $r$ dependence of $U_1$ to first order in $\rho J$, which is displayed below,

$$F_1(r)=\rho_0^2\int_D^{D_0} dD'\int_0^{D'}\frac{d\varepsilon}{D'+\varepsilon}J(\phi_D\phi_{-\varepsilon}+\phi_{-D}\phi_\varepsilon) \ . \tag{47}$$

This $r$ dependence of $F_1(r)$ has the Ruderman-Kittel-Kasuya-Yosida (RKKY) form except for a change of sign [see Ref. 17 for the justification that $F_1(r)$ represented in Eq. (47) has RKKY form]. Because of the antiferromagnetic interaction between the impurity spin and conduction-electron spin density at the impurity site, the conduction-electron spins near the impurity site tend to be antiparallel to the impurity spin and hence $F_1(r)$ is negative for small $r$. In the case of the RKKY interaction, which is induced by the conduction electrons, each impurity spin tends to be antiparallel with the conduction-electron spins around it. Therefore, two impurity spins like to be parallel when they are close, and as a consequence, the RKKY interaction [which is proportional to $(\rho_0 J)^2$ for obvious reasons] is positive when $r$ is small. In short, it is not surprising that $F_1(r)$ has a different sign from the RKKY interaction.

There are many sources of corrections that can affect simple factorization. Particle-hole symmetry breaking typically leads to small corrections, as it does not generate a new local response function which involves only impurity operators; the term involving the local response function $\langle\langle S_z;S_z\rangle\rangle$ still dominates. A similar statement may be made in regard to spatial anisotropy of the conduction band. In general, we expect the factorization to be quite robust. Even though the method we have used above fails when the initial coupling is sufficiently large that one cannot integrate out degrees of freedom until the spatial dependence has been separated out, one expects factorization to hold as long as $k_F rT/D_0 \ll 1$. The spatial dependence of $C_1$ (which is essentially the RKKY interaction), on the other hand, will depend on, for example, the high-energy part of the band structure, spatial anisotropy, etc. Recently Pollwein *et al.*[18] have calculated the response function using the $1/N$ expansion. They have verified factorization by calculating both the response function and the susceptibility and showing that they are proportional to each other at all interesting temperatures. Their calculation does not provide any insight into the mechanism for factorization. On the other hand, their method has validity for large $r$ in contrast to ours; however, they have not explored the asymptotic behavior in any detail.

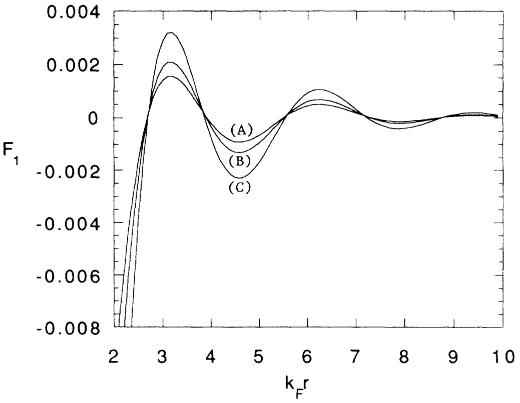

FIG. 2. The spatial dependence (first order in $J$) of the response function $\langle\langle S_z;\sigma_z(r)\rangle\rangle$, $F_1(r)$. The couplings $\rho_0 J_0$ are (A) $-0.075$, (B) $-0.10$, (C) $-0.15$.

## IV. CALCULATION OF CORRELATION FUNCTIONS

In this section we present the results of our calculation of the conduction-electron spin-density—impurity-spin correlation function $\langle \mathbf{S}\cdot\boldsymbol{\sigma}(r)\rangle$ and the conduction-electron charge density $\langle \Psi_\mu^\dagger(\mathbf{r})\Psi_\mu(\mathbf{r})\rangle$ in the spin-$\frac{1}{2}$ Kondo model. Using the procedure outlined earlier, it is straightforward to carry out the calculation. We will restrict our discussion to presenting the basic results and omit the details.

### A. Spin-spin correlation function in the Kondo model

#### *1. Perturbative scaling to separate out the spatial and thermal dependences*

In this subsection, we will discuss the conduction-electron spin-density-impurity-spin correlation function

$$C_2(\mathbf{r},T)=\langle \mathbf{S}\cdot\boldsymbol{\sigma}(r)\rangle \ .$$

For early attempts to calculate this correlation function within perturbation theory, see Refs. 13 and 19.

We begin with the following expression for the correlation function $C_2(r,T)$ ($C_2$ will not depend on the direction of $\mathbf{r}$, because the Hamiltonian is spherically symmetric):

$$C_2(r,T)=-\left[\frac{\partial}{\partial h}F\right]_{h=0} , \tag{48}$$

where $F=-k_B T\ln \mathrm{Tr}\exp[-\beta H(D_0)]$ is the free energy of the Hamiltonian, given by

$$H(D_0)=H_K(D_0)-h\mathbf{S}\cdot\boldsymbol{\sigma}(\mathbf{r}) \ . \tag{49}$$

Reducing the bandwidth from $D_0$ to $D$ as before by integrating out the electron and hole degrees of freedom with energies between $D_0$ and $D$ using second-order perturbative scaling theory leads to the effective Hamiltonian of the following form to linear order in $h$:

$$
\begin{aligned}
H(D)=\int_{\varepsilon\xi\mu}^{D}\varepsilon C^{\dagger}_{\varepsilon\xi\mu}C_{\varepsilon\xi\mu}-\tfrac{1}{2}J(D)[\Psi^{\dagger}_{\mu}(0)\boldsymbol{\sigma}_{\mu,\mu'}\Psi_{\mu'}(0)]\cdot\mathbf{S}\\
-\tfrac{1}{2}h\mathbf{S}\cdot\{J_1\Psi^{\dagger}(0)\boldsymbol{\sigma}\Psi(0)+J_t[\Psi^{\dagger}(0)\boldsymbol{\sigma}\Psi(\mathbf{r})+\Psi^{\dagger}(\mathbf{r})\boldsymbol{\sigma}\Psi(0)]+\Psi^{\dagger}(\mathbf{r})\boldsymbol{\sigma}\Psi(\mathbf{r})\}\\
+h\{K_1\Psi^{\dagger}(0)\Psi(0)+K_t[\Psi^{\dagger}(\mathbf{r})\Psi(0)+\Psi^{\dagger}(0)\Psi(\mathbf{r})]\}+U_0'+U_1'h\ .
\end{aligned}
\tag{50}
$$

The notation is similar to that used earlier. [See Sec. III after Eq. (22).]

The recursion relations for the coupling constants can be derived and are displayed below:

$$-D\frac{dJ}{dD}=-\rho_0J^2\ , \tag{51}$$

$$-D\frac{dJ_t}{dD}=-\rho_0JJ_t-\tfrac{1}{2}\rho_0J(\phi_D+\phi_{-D})\ , \tag{52}$$

$$-D\frac{dK_1}{dD}=-\tfrac{3}{8}\rho_0JJ_t(\phi_D-\phi_{-D})\ , \tag{53}$$

$$
\begin{aligned}
-D\frac{dJ_1}{dD}=-2\rho_0JJ_1-\rho_0JJ_t(\phi_D+\phi_{-D})\\
-2\rho_0JK_t(\phi_D-\phi_{-D})\ ,
\end{aligned}
\tag{54}
$$

$$-D\frac{dK_t}{dD}=-\tfrac{3}{16}\rho_0J(\phi_D-\phi_{-D})\ , \tag{55}$$

$$
\begin{aligned}
\frac{dU_1'}{dD}=\tfrac{3}{4}\rho_0^2\int_0^D\frac{d\varepsilon}{D+\varepsilon}[2J_1J+JJ_t(\phi_D+\phi_\varepsilon+\phi_{-D}+\phi_{-\varepsilon})\\
+J(\phi_D\phi_{-\varepsilon}+\phi_{-D}\phi_\varepsilon)]\ .
\end{aligned}
\tag{56}
$$

Recall that $\phi_\varepsilon=\sin(k_\varepsilon r)/k_\varepsilon r$ with $k_\varepsilon=k_F+\varepsilon/v_F$.

We integrate Eqs. (51)–(56) from $D_0$ down to $D$ such that $rD/v_F\ll 1$, and $T_K\ll D$ (see Secs. II and III), and we calculate $C_2(r,T)$ using the effective Hamiltonian at $D$. This leads to

$$
\begin{aligned}
C_2(r,T)=-U_1'(r)+\frac{1}{2}\left[J_1+2J_t\frac{\sin(k_Fr)}{k_Fr}\right.\\
\left.+\left[\frac{\sin(k_Fr)}{k_Fr}\right]^2\right]\frac{D}{D_0}\\
\times\langle\mathbf{S}\cdot\tilde{\Psi}^{\dagger}(0)\boldsymbol{\sigma}\tilde{\Psi}(0)\rangle_{H_K(D)}\ .
\end{aligned}
\tag{57}
$$

We have followed the discussion presented in Sec. III: First, we have replaced $\Psi(\mathbf{r})$ by $[\sin(k_Fr)/k_Fr]\Psi(0)$ as a result of angular averaging; second, since $k_\varepsilon r=k_Fr(1+\varepsilon/k_Fv_F)\approx k_Fr$, the correlation functions evaluated with $H_K(D)$ reduce to *local* correlation functions; third, $\Psi(0)$ is replaced by $\tilde{\Psi}(0)=\sqrt{(D_0/D)}\Psi(0)$ which is normalized. We have invoked particle-hole symmetry to eliminate the term $\langle\tilde{\Psi}^{\dagger}(0)\tilde{\Psi}(0)\rangle$. We will show below that $\langle\mathbf{S}\cdot\tilde{\Psi}^{\dagger}(0)\boldsymbol{\sigma}\tilde{\Psi}(0)\rangle$ is of the order of $\rho_0J(D)$ and, consequently, the second term is of the order of $(D/D_0)\rho_0J(D)$, while the first term is of the order of $\rho_0J(D)$. Hence, the first term dominates the second term, and we can write

$$C_2(r,T)=-U_1'(r)\ , \tag{58}$$

which is a temperature-independent function. This is yet another specific example of the general idea described earlier.

### 2. Numerical data

We have integrated the recursion relations to obtain the $r$ dependent coefficients in front of the local correlation functions in Eq. (57) and calculated the local correlation functions using Wilson's RG method (Refs. 10, 14, and 15) described in the previous section.

Calculation of the local correlation function

$$\tfrac{1}{2}\langle\mathbf{S}\cdot\tilde{\Psi}^{\dagger}(0)\boldsymbol{\sigma}\tilde{\Psi}(0)\rangle\equiv\langle\mathbf{S}\cdot\boldsymbol{\sigma}(0)\rangle$$

using the nonperturbative RG method is relatively simple compared to the calculation of the response function. We can use Wilson's original diagonalization procedure in each subspace $(Q,S^2,m_S)$. The corresponding second-order perturbation (in $H_{NI}$) is worked out in Appendix A. Again, the second-order perturbation contribution to the local correlation function is small compared to that for the susceptibility in Wilson's procedure. Therefore, we take $\bar{\beta}$ large, and we need only keep a few energy states to maintain good accuracy. We use $\Lambda=3$ and the same set of $\bar{\beta}$ ($\bar{\beta}=1.501$, 1.308, 1.140, 0.994, and 0.867) as we did in calculating the response function. It turns out to be sufficient to retain about 120 states in this case.

We have calculated both $\langle\mathbf{S}\cdot\boldsymbol{\sigma}(0)\rangle_{H_K(D_0)}$ with the initial Hamiltonian and $\langle\mathbf{S}\cdot\boldsymbol{\sigma}(0)\rangle_{H_K(D)}$ with the renormalized Hamiltonian. We have computed this correlation function for $\rho_0J_0(D_0)=-0.075$, $-0.1$, and $-0.15$, with corresponding Kondo temperatures (in units of $D_0$) $4.93\times10^{-4}$, $1.44\times10^{-5}$, and $4.11\times10^{-7}$, respectively. $D$ is taken to be $10^{-2}D_0$. For $k_Fr\le 10$, the conditions for $D$ discussed in the previous sections ($T,T_K\ll D$ and $k_Fr\ll D_0/D$) are satisfied. The result for this local correlation is shown in Fig. 3.

From these curves, one can see that $\langle\mathbf{S}\cdot\boldsymbol{\sigma}(0)\rangle_{H_K(\bar{D})}$ ($\bar{D}=D_0$ or $D$) approaches a constant very quickly when the temperature is lowered. The crossover to a constant occurs around $T\approx\bar{D}/10$. It is clear that this constant depends on the initial coupling, and, hence, we can write

$$\langle\mathbf{S}\cdot\boldsymbol{\sigma}(0)\rangle_{H_K(\bar{D})}=c_2(\rho_0J(\bar{D})) \tag{59}$$

for $T<\bar{D}/10$. The values of $c_2(\rho_0J(\bar{D}))$ are listed in Table II.

In Table II, we display the values for $c_2$ for two sets of coupling constants: one is for $\rho_0J_0=-0.15$, $-0.10$, and $-0.075$ with cutoff $D_0$, and the other set is obtained by integrating the recursion relations (to second-order) down to $D=D_0/100$, i.e., $\rho_0J(\bar{D}=D)=-0.485$, $-0.185$, and $-0.114$, respectively. The values are calculated exactly

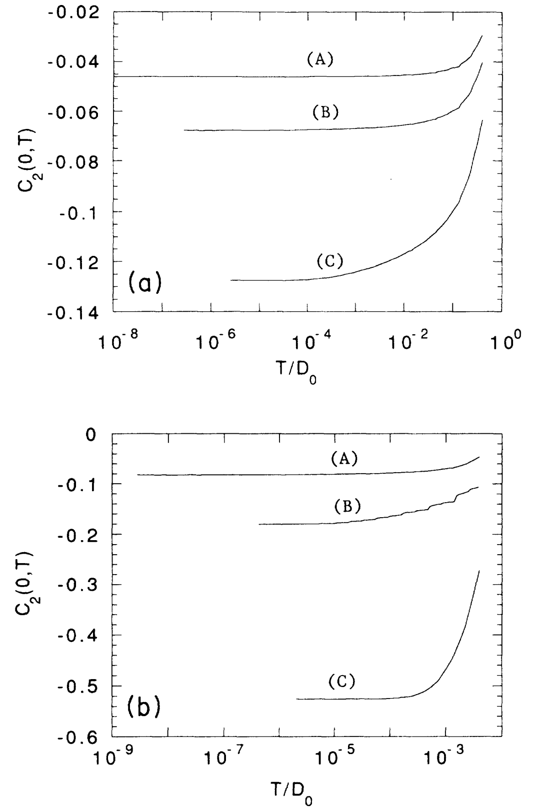

FIG. 3. (a) The local spin correlation function $\langle \mathbf{S}\cdot\boldsymbol{\sigma}(\mathbf{r})\rangle$ as a function of temperature (in units of $D_0$) for $\rho_0 J(\bar{D})=$(A) $-0.075$, (B) $-0.10$, (C) $-0.15$ at $\bar{D}=D_0$. (b) The local spin correlation function $\langle \mathbf{S}\cdot\boldsymbol{\sigma}(\mathbf{r})\rangle$ as a function of temperature (in units of $D_0$) for the corresponding renormalized coupling at $\bar{D}=D=D_0/100$ for $\rho_0 J(\bar{D})=$(A) $-0.114$, (B) $-0.185$, (C) $-0.485$.

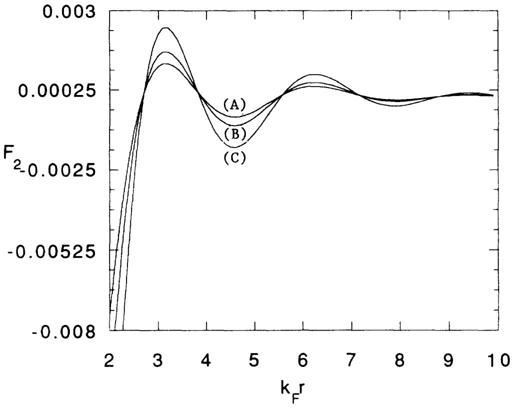

FIG. 4. The spatial dependence (first order in $J$) of the correlation function $\langle \mathbf{S}\cdot\boldsymbol{\sigma}(\mathbf{r})\rangle$, $F_2$. The coupling constants are (A) $-0.075$, (B) $-0.010$, (C) $-0.15$.

using Wilson's RG method given $\rho_0 J(\bar{D})$ (where $\bar{D}=D_0$ or $D$). For comparison we present $c_2'=-U_1'(0)$ evaluated using second-order scaling equations [see Eqs. (51)–(58)]. Note that, for small $\rho_0 J(\bar{D})$, the differences are only about 10%. We also investigate the proportionality of $c_2$ to $\rho_0 J(\bar{D})$. From the values in the table for $c_2[\rho_0 J(D)]$, we find

$$c_2/[\rho_0 J(D)]=c_{20}+c_{21}\rho_0 J(D)$$

with $c_{20}\approx-0.40$ and $c_{21}\approx-3.0$. In this case the second-order contributions are quite significant.

The results for $\langle \mathbf{S}\cdot\boldsymbol{\sigma}(r)\rangle$ at zero temperature are plotted in Fig. 4. In these figures, we have only plotted the first-order contribution to $\langle \mathbf{S}\cdot\boldsymbol{\sigma}(r)\rangle$, which we denote as $F_2(r)$,

$$F_2(r)=\tfrac{3}{4}\rho_0^2\int_D^{D_0}dD'\int_0^D\frac{d\varepsilon}{D'+\varepsilon}J(\phi_{D'}\phi_{-\varepsilon}+\phi_{-D'}\phi_{\varepsilon}) \; . \tag{60}$$

It also has the RKKY form (apart from a minus sign) as explained in Ref. 17. Therefore, the correlation function $\langle \mathbf{S}\cdot\boldsymbol{\sigma}(\mathbf{r})\rangle$ and the zero-frequency response function $\langle\langle S_z;\sigma_z(\mathbf{r})\rangle\rangle$ have the same spatial dependence in leading order. However, their temperature dependences are dramatically different.

### B. Conduction electron charge density in the Kondo model

#### 1. *Perturbative scaling to separate out the spatial and temperature dependences*

We begin with the following expression for the correlation function:

$$C_3(r,T)=\langle \Psi_\mu^\dagger(\mathbf{r})\Psi_\mu(\mathbf{r})\rangle_{H_K(D_0)}=-\left[\frac{\partial}{\partial h}F\right]_{h=0} , \tag{61}$$

where $F=-k_B T\ln\mathrm{Tr}\exp[-\beta H(D_0)]$ is the free energy of the Hamiltonian given by

$$H(D_0)=H_K(D_0)-h\Psi_\mu^\dagger(\mathbf{r})\Psi_\mu(\mathbf{r}) \; . \tag{62}$$

The most general effective Hamiltonian at cutoff $D$ within second-order scaling theory assumes the following form to linear order in $h$:

TABLE II. Values of $c_2(\rho_0 J(\bar{D}))$ at low temperatures for two sets of coupling at $\bar{D}=D_0$ and $\bar{D}=D$. The corresponding values from perturbative scaling are also listed for comparison.

| | Bandwidth $D_0$ | | | Bandwidth $D$ | | |
|---|---|---|---|---|---|---|
| $\rho_0 J(\bar{D})$ | $-0.075$ | $-0.10$ | $-0.15$ | $-0.114$ | $-0.185$ | $-0.485$ |
| $c_2$ | $-0.0461$ | $-0.0679$ | $-0.128$ | $-0.0823$ | $-0.179$ | $-0.526$ |
| $c_2/\rho_0 J(\bar{D})$ | 0.615 | 0.679 | 0.853 | 0.722 | 0.968 | 1.08 |
| $c_2'$ | $-0.0501$ | $-0.0755$ | $-0.167$ | | | |

$$H(D)=\int_{\varepsilon\xi\mu}^{D}\varepsilon C^{\dagger}_{\varepsilon\xi\mu}C_{\varepsilon\xi\mu}-\tfrac{1}{2}J(D)[\Psi^{\dagger}_{\mu}(0)\sigma_{\mu,\mu'}\Psi_{\mu'}(0)]\cdot\mathbf{S}-\tfrac{1}{2}h\mathbf{S}\cdot\{J_1\Psi^{\dagger}(0)\sigma\Psi(0)+J_t[\Psi^{\dagger}(0)\sigma\Psi(\mathbf{r})+\Psi^{\dagger}(\mathbf{r})\sigma\Psi(0)]\}$$
$$-h[K_1\Psi^{\dagger}(0)\Psi(0)+\Psi^{\dagger}(\mathbf{r})\Psi(\mathbf{r})]+U_0''+U_1''h\ . \tag{63}$$

The recursion relations for the coupling constants can be derived as usual and are given below:

$$-D\frac{dJ}{dD}=-\rho_0 J^2\ , \tag{64}$$

$$-D\frac{dJ_t}{dD}=-\rho_0 J_t+\rho_0 J(\phi_D-\phi_{-D})\ , \tag{65}$$

$$-D\frac{dK_1}{dD}=\tfrac{3}{8}\rho_0 J_t(\phi_D-\phi_{-D})\ , \tag{66}$$

$$-D\frac{dJ_1}{dD}=-2\rho_0 J_1-\rho_0 J_t(\phi_D+\phi_{-D})\ , \tag{67}$$

$$\frac{dU_1''}{dD}=\tfrac{3}{4}\rho_0^2\int_0^D\frac{d\varepsilon}{D+\varepsilon}[2J_1J+J_t(\phi_D+\phi_\varepsilon+\phi_{-D}+\phi_{-\varepsilon})]\ . \tag{68}$$

Now we calculate the charge density $C_3(r,T)$ with the effective Hamiltonian $H(D)$, and we obtain,

$$C_3(r,T)=-U_1''(r)+\frac{1}{2}\left[J_1+2J_t\frac{\sin(k_Fr)}{k_Fr}\right]\frac{D}{D_0}$$
$$\times\langle\mathbf{S}\cdot\tilde{\Psi}^{\dagger}(0)\sigma\tilde{\Psi}(0)\rangle_{H_K(D)}\ . \tag{69}$$

We have invoked particle-hole symmetry to eliminate the term $\langle\tilde{\Psi}^{\dagger}(0)\tilde{\Psi}(0)\rangle$. It is clear that the second term is down by a factor of $D/D_0$ compared to the first term. Thus, $C_3(r,T)$ is temperature independent and is simply $-U_1''(r)$.

### 2. Numerical data and discussion

The spatial dependence of the charge density

$$\rho(r)=-U_1''(r)$$

is plotted in the Fig. 5. From the recursion relations, one can see that the leading-order contribution to the charge density is second order in the coupling constant $\rho_0 J_0$ which is small as shown in the figure. However, our leading-order (second-order) result is not exact due to the neglect of the energy dependence of the coupling constants (particularly in $J_x$). We believe that inclusion of the energy dependences of the coupling constants will not change the qualitative conclusions.

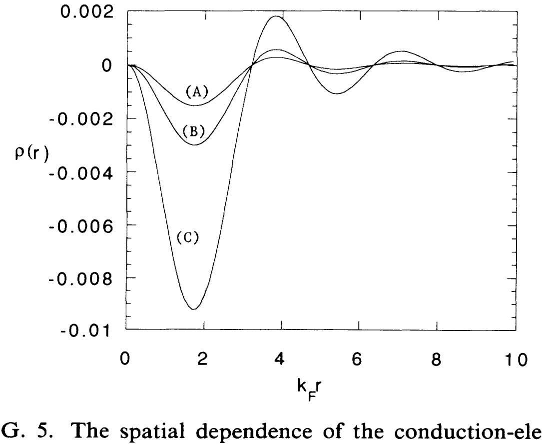

FIG. 5. The spatial dependence of the conduction-electron charge density $\rho(r)$. The coupling constants are (A) $-0.075$, (B) $-0.10$, (C) $-0.15$.

Our main conclusion is that the charge density is independent of the temperature. The Kondo effect does not show up in the conduction-electron charge density at this level. However, for an impurity system which has a high Kondo temperature, the above conclusion may not be valid. In that case, $D$ cannot be sufficiently small (but still $D\gg T_K$ in order that the perturbative scaling be valid) so that the second term (temperature-dependent term) cannot be neglected. This is the case for *Al*Mn, and *Al*Cr, where the Kondo temperatures are about 530 and 1200 K, respectively. In this case, the temperature and spatial dependences are complicated and one does not expect the factorization of the temperature and spatial dependences.[20,21]

As far as the spatial dependence is concerned, one can see clearly the usual $2k_Fr$ oscillation. Due to the limited range of $k_Fr$, we cannot see the power-law dependence of the amplitude of the oscillation. In addition, because we do not know the large-$r$ asymptotic behavior for the Kondo model (our method is only valid for $k_Fr\ll D_0/D$ and $T,T_K\ll D$), we do not know if there is suppression of the charge-density oscillation near the impurity. These topics remain to be investigated. It is more interesting to examine the charge density in the asymmetric Anderson model and examine the charge-density oscillations. We have done so using the same formalism, and we have found that in various regimes (in particular, the mixed-valence regime) the amplitude of charge-density oscillation around the impurity depends strongly on the impurity energy level $\varepsilon_d$. We also found that when the system goes from the mixed-valence regime to the Kondo regime as $\varepsilon_d$ is varied, the corresponding charge-density variations are suppressed significantly. This will be reported elsewhere.

## V. MODELS WITH HIGHER-SPIN IMPURITIES

We now comment on how the mechanism for factorization that we have outlined for the spin-$\frac{1}{2}$ problem can be carried over to more realistic models. A commonly occurring situation is one in which the orbital angular momentum of the impurity is zero: this is the case for Mn impurities in Cu where $\mathrm{Mn}^{++}$ is an $S$-state ion with $S=\frac{5}{2}$. The assumption of zero orbital angular momentum $\mathbf{L}$ is also a reasonable approximation when crystal-field effects quench $\mathbf{L}$ as appears to be the case for Fe in Cu. The appropriate Hamiltonian is then given by

$$H_K = -J \sum_{m,\varepsilon,\varepsilon'} \mathbf{S}\cdot c^{\dagger}_{\varepsilon m\mu} \frac{\sigma_{\mu\mu'}}{2} c_{\varepsilon' m\mu'} \ , \tag{70}$$

where the sum over $m$ runs over the number of angular momentum channels of the conduction electron which we take to be precisely $2S$ where $S$ is the spin impurity. In the case when the number of channels $n$ is $2S$, the impurity moment is quenched and Fermi-liquid behavior is obtained at low temperatures; the case $n > 2S$ leads to non-Fermi-liquid behavior and we will not discuss it here. By an application of the Schrieffer-Wolff transformation[22] to the appropriate Anderson Hamiltonian, the coupling constant $J$ can be shown to be inversely proportional to $S$.[23]

Consider applying the procedure outlined in the earlier sections to the calculation of a correlation function at some distance $\mathbf{r}$ for the Hamiltonian given above. We first apply perturbative scaling to reduce the cutoff from $D_0$ to $D$ such that $rD/\hbar v_F \ll 1$. This leads to a sum of products of functions of $r$ and local correlation functions that have the same symmetry as the correlation function under consideration. Note that there is a natural hierarchy of operators as explained earlier: terms with $n$ conduction-electron operators will be accompanied by a factor of $(D/D_0)^{n/2}$ and will be small. Terms composed entirely of impurity operators will thus dominate and one need only form operators with the right symmetry properties. Consider the calculation of the response function $C_1(r,T)$ discussed in Sec. III for $S=2$. We will obtain, in addition to the identity operator and $\langle\langle S_z;S_z\rangle\rangle$, a term, for example, of the form $\langle\langle S_z;S_z^3\rangle\rangle$. Recall that we have argued that a perturbative scaling calculation provides a good estimate of the order of magnitude of various response functions. Therefore, in order to estimate the importance of this additional term we have evaluated the zero-frequency response function $\langle\langle S_z;S_z^3\rangle\rangle$ to leading logarithmic order in perturbation theory. This straightforward calculation yields the result

$$\langle\langle S_z;S_z^3\rangle\rangle / \langle\langle S_z;S_z\rangle\rangle = \tfrac{34}{5} \ . \tag{71}$$

For arbitrary $S$ the ratio is $\langle\langle S_z;S_z^3\rangle\rangle_0 / \langle\langle S_z;S_z\rangle\rangle_0$, where $\langle\ \rangle_0$ denotes a free-spin average. Note, however, that the term proportional to $\langle\langle S_z;S_z^3\rangle\rangle$ is accompanied by an extra factor of $(\rho J)^2$ in the expression for $C_1(\mathbf{r},T)$ since it appears in higher order in the perturbative scaling expansion. Thus, when $T_K \ll D_0$ and, hence, $\rho J$ is small, the term $\langle\langle S_z;S_z\rangle\rangle$, which is the susceptibility, dominates. For example, if $\rho J = 0.1$, the term proportional to $\langle\langle S_z;S_z^3\rangle\rangle$ will be of order 10% of the term proportional to the susceptibility. Similar arguments apply for higher spin and the scaling $J \propto (1/S)$ alluded to earlier ensures that the other terms remain quantitatively small for small $\rho J$. Thus, the factorization of the Knight shift argued to hold for the spin-$\frac{1}{2}$ problem can be expected to be valid for more general Hamiltonians relevant to transition metal impurities with calculable corrections.

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## APPENDIX A: SECOND-ORDER PERTURBATION CALCULATION OF $\langle \hat{A} \rangle$

In the appendix, we give the second-order perturbation formalism for calculating the average $\langle \hat{A} \rangle$. We consider the case that $\hat{A}$ commutes with the total spin and charge, but not necessarily the Hamiltonian itself. We write the total Hamiltonian as

$$H = H_N + H_B + H_I \ , \tag{A1}$$

where

$$H_N = \Lambda^{(N-1)/2} \left[ \sum_{n=0}^{N} \Lambda^{-n/2} \xi_n ( f^{\dagger}_{n\mu} f_{n+1\mu} + f^{\dagger}_{n+1\mu} f_{n\mu} ) - \tilde{J} f^{\dagger}_{0\mu} \tfrac{1}{2} \boldsymbol{\sigma}_{\mu,\mu'} f_{0\mu'} \cdot \mathbf{S} \right] , \tag{A2}$$

$$H_B = \Lambda^{(N-1)/2} \left[ \sum_{n=N+1}^{M-1} \Lambda^{-n/2} \xi_n ( f^{\dagger}_{n\mu} f_{n+1\mu} + \mathrm{H.c.} ) \right] , \tag{A3}$$

$$H_I = \Lambda^{1/2} ( f^{\dagger}_{N\mu} f_{N+1\mu} + \mathrm{H.c.} ) \ . \tag{A4}$$

We want to calculate

$$\langle \hat{A} \rangle = \frac{\mathrm{Tr}[\hat{A} \exp(-\bar{\beta} H)]}{\mathrm{Tr} \exp(-\bar{\beta} H)} \ .$$

This involves evaluating the traces to second order in $H_I$. Define

$$Z = \mathrm{Tr} \exp(-\bar{\beta} H) \ , \tag{A5}$$

$$Y = \mathrm{Tr}[\hat{A} \exp(-\bar{\beta} H)] \ . \tag{A6}$$

We will use the following well-known identity:

$$e^{-\bar{\beta}(H_0 + H_I)} = e^{-\bar{\beta} H_0} T \exp\left[ -\int_0^{\bar{\beta}} d\lambda\, H_I(\lambda) \right] , \tag{A7}$$

where $T$ denotes ordering with respect to $\lambda$ and

$$H_I(\lambda) = e^{\lambda H_0} H_I e^{-\lambda H_0} \ . \tag{A8}$$

The partition function can be written as

$$Z = Z^{(0)} + Z^{(2)} \tag{A9}$$

where $Z^{(0)} = \mathrm{Tr} e^{\bar{\beta} H_0}$ with $H_0 = H_N + H_B$. $Z^{(2)}$ is the second-order contribution to the partition function, which has been calculated in Appendix F in Ref. 14. We simply quote the result here:

$$Z^{(2)}/Z^{(B)} = \frac{\bar{\beta}}{\Lambda} \sum_{\kappa,\kappa'} n_S | \langle k \| f^{\dagger}_N \| k' \rangle |^2 e^{-\bar{\beta} E} u(E - E') \ , \tag{A10}$$

where $n_S = 2S+1$, $k$ denotes the state $(Q, S^2, r)$, i.e., the

$r$th state in the subspace with quantum numbers $Q$ and $S^2$, with energy $E$, and $k'$ denotes state $(Q',S'^2,r')$ with energy $E'$. The function $u(\delta E)$ is defined by

$$u(\delta E)=\sum_j \frac{v_j^2}{1+e^{-\bar\beta\varepsilon_j}}\frac{e^{\bar\beta(\delta E-\varepsilon_j)}-1}{\delta E-\varepsilon_j}\ , \tag{A11}$$

where $\{\varepsilon_j,v_j\}$ are obtained from the diagonalization of $H_B$.

$$H_B=\sum_j \varepsilon_j a_{j\mu}^\dagger a_{j\mu}\ , \tag{A12}$$

$$f_{N+1\mu}=\sum_j v_j a_j\ . \tag{A13}$$

The following is devoted to the calculation of

$$Y=\mathrm{Tr}(e^{-\bar\beta H}\hat A)=Y^{(0)}+Y^{(2)}\ ,$$

where $Y^{(0)}$ and $Y^{(2)}$ are zeroth- and second-order contributions, respectively. Because $\hat A$ does not commute with $H_N$, the calculation is a little bit involved. $Y^{(2)}$ can be written as follows:

$$\begin{aligned}Y^{(2)}&=\mathrm{Tr}\left[e^{-\beta BH_N}e^{-\bar\beta H_B}T\left[\int_0^{\bar\beta}d\lambda\, H_I(\lambda)\int_0^{\bar\lambda}d\lambda' H_I(\lambda')\hat A\right]\right]\\&=\frac{Z^{(0)}}{\Lambda}\sum_{\mu,\nu}\int_0^{\bar\beta}d\lambda\int_0^{\lambda}d\lambda'[\langle f_{N\mu}^\dagger(\lambda)f_{N\nu}(\lambda')\hat A\rangle_N\langle f_{N+1\mu}(\lambda)f_{N+1\nu}^\dagger(\lambda')\rangle_B\\&\qquad+\langle f_{N\mu}(\lambda)f_{N\nu}^\dagger(\lambda')\hat A\rangle_N\langle f_{N+1\mu}^\dagger(\lambda)f_{N+1\nu}(\lambda')\rangle_B]\ ,\end{aligned} \tag{A14}$$

where $\langle\ \rangle_n$ and $\langle\ \rangle_B$ are the average in the subspaces defined by $H_N$ and $H_B$, respectively.

### 1. Evaluation of the trace involving $H_N$

We can write

$$\begin{aligned}\mathrm{Tr}[e^{-\bar\beta H_N}f_{N\mu}^\dagger(\lambda)f_{N\nu}(\lambda')\hat A]=\sum_{k,k',k''}\sum_{m_S,m_S'm_S''}&e^{-\beta E}\langle k\|f_N^\dagger(\lambda)\|k'\rangle\langle S',m_S';\tfrac12,\mu|S,m_S\rangle\\&\times\langle k'\|f_N(\lambda')\|k''\rangle\langle S',m_S';\tfrac12,\nu|S'',m_S''\rangle\langle k''\|\hat A\|k\rangle\ ,\end{aligned} \tag{A15}$$

where $k$, $k'$, $k''$ denote eigenstates of $H_N$: $|Q,S^2,r\rangle$, $|Q',S''^2,r'\rangle$, and $|Q,S^2,r''\rangle$ with energies $E$, $E'$, and $E''$, respectively. Because $\hat A$ commutes with total spin and charge operators, $|k\rangle,|k''\rangle$ lie in the same (charge, spin) subspace. similarly, we have

$$\begin{aligned}\mathrm{Tr}[e^{-\bar\beta H_N}f_{N\mu}(\lambda)f_{N\nu}^\dagger(\lambda')\hat A)]=\sum_{k,k',k''}\sum_{m_S,m_S'}&e^{-\beta E}\langle k\|f_N(\lambda)\|k'\rangle\langle S,m_S;\tfrac12,\mu|S,m_S\rangle\\&\times\langle k'\|f_N^\dagger(\lambda')\|k''\rangle\langle S,m_S;\tfrac12,\nu|S',m_S\rangle\langle k''\|\hat A\|k\rangle\ .\end{aligned} \tag{A16}$$

### 2. Trace involving $H_B$

From Appendix F in Ref. 14, it is easy to show that

$$\langle f_{N+1\mu}(\lambda)f_{N+1\nu}^\dagger(\lambda')\rangle_B=\delta_{\mu\nu}\sum_j v_j^2 e^{-(\lambda-\lambda')\varepsilon_j}\frac{1}{1+e^{-\bar\beta\varepsilon_j}}\ , \tag{A17}$$

$$\langle f_{N+1\mu}^\dagger(\lambda)f_{N+1\nu}(\lambda')\rangle_B=\delta_{\mu\nu}\sum_j v_j^2 e^{(\lambda-\lambda')\varepsilon_j}\frac{e^{-\bar\beta\varepsilon_j}}{1+e^{-\bar\beta\varepsilon_j}}\ . \tag{A18}$$

### 3. Summation over spin indices

Now, combine all equation from Eqs. (A15) to (A18), and sum over $\mu,\nu,m_S,m_S'$. We have

$$\begin{aligned}Y^{(2)}=\frac{Z^{(B)}}{\Lambda}\int_0^{\bar\beta}d\lambda\int_0^{\lambda}d\lambda'\sum_{k,k'k''}&\left[e^{-\bar\beta E}\langle k\|f_N^\dagger(\lambda)\|k'\rangle\langle k'\|f_N(\lambda')\|k''\rangle\langle k''\|\hat A\|k\rangle n_S\sum_j v_j^2 e^{-(\lambda-\lambda')\varepsilon_j}\frac{1}{1+e^{-\bar\beta\varepsilon_j}}\right.\\&\left.+e^{-\bar\beta E}\langle k\|f_N(\lambda)\|k'\rangle\langle k'\|f_N^\dagger(\lambda')\|k''\rangle\langle k''\|\hat A\|k\rangle n_{S'}\sum_j v_j^2 e^{(\lambda-\lambda')\varepsilon_j}\frac{e^{-\bar\beta\varepsilon_j}}{1+e^{-\bar\beta\varepsilon_j}}\right]\ .\end{aligned} \tag{A19}$$

Changing $\varepsilon_j \rightarrow -\varepsilon_j$ in the summation over $j$ in the second term in the bracket ($M-N$ is taken to be odd in our calculation, consequently, $v_j = v_j$ and $\varepsilon_j = -\varepsilon_{-j}$), and extracting the common factors, we obtain

$$Y^{(2)} = \frac{Z^{(B)}}{\Lambda} \int_0^{\bar{\beta}} d\lambda \int_0^{\lambda} d\lambda' \sum_{k,k'k''} e^{-\bar{\beta}E} e^{\lambda(E-E')} e^{\lambda'(E'-E'')} \times \sum_j v_j^2 e^{-(\lambda-\lambda')\varepsilon_j} \frac{1}{1+e^{-\bar{\beta}\varepsilon_j}} \times \langle k'' \| \hat{A} \| k \rangle ( n_S \langle k \| f_N^\dagger \| k' \rangle \langle k'' \| f_N^\dagger \| k' \rangle + n_{S'} \langle k' \| f_N^\dagger \| k \rangle \langle k' \| f_N^\dagger \| k'' \rangle ) , \tag{A20}$$

where we have substituted the expressions for $f_N(\lambda)$, $f_N^\dagger(\lambda')$:

$$f_N(\lambda) = e^{\lambda H_0} f_N e^{-\lambda H_0} , \text{ etc.}$$

### 4. Integration over $\lambda, \lambda'$

The integration over $\lambda$ and $\lambda'$ can be performed easily obtaining the following expression for $Y^{(2)}$:

$$Y^{(2)} = \frac{Z^{(B)}}{\Lambda} \sum_{k,k',k''} \frac{1}{E-E''} [ e^{-\bar{\beta}E''} u(E''-E') - e^{-\bar{\beta}E} u(E-E') ] \times \langle k'' \| \hat{A} \| k \rangle [ n_S \langle k \| f_N^\dagger \| k' \rangle \langle k'' \| f_N^\dagger \| k' \rangle + n_{S'} \langle k' \| f_N^\dagger \| k \rangle \langle k' \| f_N^\dagger \| k'' \rangle ] . \tag{A21}$$

Now the second-order contribution of $\hat{A}$ can be obtained as follows:

$$\begin{aligned} \langle \hat{A} \rangle &= ( Y^{(0)} + Y^{(2)} ) / ( Z^{(0)} + Z^{(2)} ) + \text{higher-order terms} \\ &= Y^{(0)}/Z^{(0)} + Y^{(2)}/Z^{(0)} - ( Y^{(0)}/Z^{(0)} ) Z^{(2)}/Z^{(0)} + \text{higher-order terms} . \end{aligned} \tag{A22}$$

In this equation, the first term is the zeroth-order contribution and the second and third terms constitute the second-order contribution.

In the actual calculation, we tabulate $u(\delta E)$ and the corresponding derivative $u'(\delta E)$ [$u'(\delta E)$ is needed to calculate those terms in the final expression for $Y^{(2)}$ in which $E = E''$] and use simple linear interpolation.

## APPENDIX B: RG PROCEDURE IN THE SUBSPACE $(Q, m_S)$

### 1. Iterative diagonalization in the subspace $(Q, m_S)$

When we calculate $\langle\langle S_z ; \sigma_z(0) \rangle\rangle$, we need to calculate the average $\langle \sigma_z(0) \rangle_H$ (see Sec. IV), where

$$H = H_K - hS_z . \tag{B1}$$

The total spin of the Hamiltonian $H$ is no longer conserved. Therefore, we have to diagonalize the Hamiltonian in subspace $(Q, m_S)$ instead of $(Q, S^2, m_S)$. However, the basic structure of the procedure remains the same; thus, we follow closely Appendix B in Ref. 14.

Let $\{ |Q, m_S, r\rangle \}$ denote the eigenstates of $H_N$ with charge $Q$ and $z$ component of spin $m_S$. The recursive procedure generates new states due to the addition of the operators $f_{N+1\uparrow}^\dagger$ and $f_{N+1\downarrow}^\dagger$. We define basis states of $H_{N+1}$ that are eigenstates of $Q_{N+1}$, $S_{N+1z}$ as follows:

$$\begin{aligned} |Q, m_S, r, 1\rangle_{N+1} &= |Q+1, m_S, r\rangle_N , \\ |Q, _S, r, 2\rangle_{N+1} &= f_{N+1\uparrow}^\dagger |Q, m_S - \tfrac{1}{2}, r\rangle_N , \\ |Q, m_S, r, 3\rangle_{N+1} &= f_{N+1\downarrow}^\dagger |Q, m_S + \tfrac{1}{2}, r\rangle_N , \\ |Q, m_S, r, 4\rangle_{N+1} &= f_{N+1\uparrow}^\dagger f_{N+1\downarrow}^\dagger |Q-1, m_S, r\rangle_N . \end{aligned} \tag{B2}$$

These basis states are the eigenstates of $H_N$ with eigenvalues $E_N(Q+1, m_S, r)$, $E_N(Q, m_S - \frac{1}{2}, r)$, $E_N(Q, m_S + \frac{1}{2}, r)$, and $E_N(Q-1, m_S, r)$, respectively. The recursion relation is given by

$$H_{N+1} = \Lambda^{1/2} H_N + \xi_N H_{NI} . \tag{B3}$$

The diagonal matrix elements of $H_{N+1}$ are given by those of $H_N$, and the off-diagonal parts are given by those of $H_{NI}$. The only nonvanishing matrix elements of $H_{NI}$ are given by

$$\langle Q, m_S, r', 1 | H_{NI} | Q, m_S, r, 2 \rangle = \langle Q+1, m_S, r' | f_{N\uparrow}^\dagger | Q, m_S - \tfrac{1}{2}, r \rangle ,$$

$$\langle Q, m_S, r', 1 | H_{NI} | Q, m_S, r, 3 \rangle = \langle Q+1, m_S, r' | f_{N\downarrow}^\dagger | Q, m_S + \tfrac{1}{2}, r \rangle ,$$

$$\langle Q, m_S, r', 2 | H_{NI} | Q, m_S, r, 4 \rangle = \langle Q, m_S - \tfrac{1}{2}, r' | f_{N\downarrow}^\dagger | Q-1, m_S, r \rangle ,$$

$$\langle Q,m_S,r',3|H_{NI}|Q,m_S,r,4\rangle = -\langle Q,m_S+\tfrac{1}{2},r'|f_{N\uparrow}^{\dagger}|Q-1,m_S,r\rangle \ .$$

This completes the set up of the matrix elements of $H_{N+1}$ in subspace $(Q,m_S)$. Diagonalization of this matrix gives a set of eigenstates of $H_{N+1}$ which are related to the old basis set defined in Eq. (B2) by a unitary transformation given by

$$|Q,m_S,\omega\rangle = \sum_{i,r} U_{Qm_S}(\omega,r,i)|Q,m_S,r,i\rangle \ . \tag{B4}$$

The corresponding eigenenergy is $E_{N+1}(Q,m_S,r,i)$. Knowing $U_{Qm_S}(\omega,r,i)$, we can calculate the matrix elements of $f_{N+1}^{\dagger}$ in the basis formed by the eigenstates of $H_{N+1}$. It is easy to verify that

$$\langle Q,m_S,\omega|f_{N+1\mu}^{\dagger}|Q',m_{S'}\omega'\rangle = \sum_r [U_{Qm_S}(\omega,r,k)U_{Q'S_z'}(\omega',r,1)\pm U_{Qm_S}(\omega,r,4)U_{Q'S_z'}(\omega',r,k')] \ , \tag{B5}$$

where the + sign, $k=2$, and $k'=3$ are used if $m_S=m_S=m_S'+\frac{1}{2}$, $\mu=\frac{1}{2}$; the − sign, $k=3$, and $k'=2$ are used if $m_S=m_S'-\frac{1}{2}$, $\mu=-\frac{1}{2}$.

### 2. Second-order perturbation formalism for $\langle \hat{A} \rangle$

We now simply state the result of the second-order perturbation calculation of $\langle \hat{A} \rangle$ when only $Q$ and $m_S$ but not $S^2$ are good quantum numbers [e.g., in the case when the Hamiltonian given by Eq. (1)] since the derivation is completely parallel to that in Appendix A. The partition function can be written as

$$Z=Z^{(0)}+Z^{(2)} \ , \tag{B6}$$

$$Z^{(0)}=Z_N Z_B \ . \tag{B7}$$

The notation is same as that in Appendix A, except we have replaced $H_N$ by $H_N-\tilde{h}S_z$ $(\tilde{h}=R_N h =[2/(1+\Lambda^{-1})]\Lambda^{(N-1)/2}h$, where $R_N$ is the rescaling factor defined in Sec. III). $Z^{(2)}$ is given by

$$Z^{(2)}=\frac{\bar{\beta}}{\Lambda}Z_B \sum_{Q,m_S,\mu} \sum_{r,r'} |\langle Q,m_S,r|f_{N\mu}^{\dagger}|Q-1,m_S-\mu,r'\rangle|^2 \times u(E-E')e^{-\bar{\beta}E} \ . \tag{B8}$$

Let $\langle \hat{A} \rangle_N$ denote the average value evaluated with $H_N$ (the zeroth-order contribution). Then, to second order in perturbation theory, we have

$$\langle \hat{A} \rangle = \langle \hat{A} \rangle_N + \frac{Y^{(2)}}{Z^{(0)}} - \langle \hat{A} \rangle_N \frac{Z^{(2)}}{Z^{(0)}} \ , \tag{B9}$$

where $Y^{(2)}$ is given by

$$\begin{aligned} Y^{(2)}=\frac{Z^{(B)}}{\Lambda} \sum_{Q,m_S,\mu} \sum_{r,r',r''} \frac{1}{E-E''}[e^{\bar{\beta}E''}u(E''-E')-E^{\bar{\beta}E}u(E-E')]\langle Q,m_S,r''|\hat{A}|Q,m_S,r\rangle \\ \times[\langle Q,m_S,r''|f_{N\mu}^{\dagger}|Q-1,m_S-\mu,r'\rangle\langle Q,m_S,r|f_{N\mu}^{\dagger}|Q-1,m_S+\mu,r'\rangle \\ +\langle Q+1,m_S+\mu,r'|f_{N\mu}^{\dagger}|Q,m_S,r\rangle\langle Q+1,m_S+\mu,r'|f_{N\mu}^{\dagger}|Q,m_S,r''\rangle] \ . \end{aligned} \tag{B10}$$

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[1]Kan Chen, C. Jayaprakash, and H. R. Krishnamurthy, Phys. Rev. Lett. **58**, 929 (1987), and references therein.

[2]V. T. Rajan, J. H. Lowenstein, N. Andrei, Phys. Rev. Lett. **49**, 497 (1982); N. Andrei, K. Furuya, and J. H. Lowenstein, Rev. Mod. Phys. **55**, 331 (1983); A. M. Tsevelick and P. B. Wiegmann, Adv. Phys. **32**, 453 (1983).

[3]P. B. Colemna, Phys. Rev. B **29**, 3035 (1984).

[4]N. E. Bickers, Rev. Mod. Phys. **59**, 845 (1987), and references therein.

[5]D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [Sov. Phys. Usp. **3**, 320 (1960)].

[6]T. J. Aton, T. S. Stakelon, and C. P. Slichter, Phys. Rev. B **21**, 4060 (1980).

[7]J. E. Gubernatis, *Quantum Monte Carlo Methods in Equilibrium and Nonequilibrium Systems*, in Proceedings of the Ninth Taniguchi International Symposium (Springer-Verlag, Berlin, 1987), p. 114.

[8]D. Šokčević, V. Zlatić, and B. Horvatić, Phys. Rev. B **39**, 603 (1989).

[9]H. R. Krishna-murthy and C. Jayaprakash, Phys. Rev. B **30**, 2806 (1984).

[10]K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).

[11]P. W. Anderson, J. Phys. C **3**, 2436 (1970).

[12]C. Itzykson and J.-B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).

[13]E. Müller-Hartmann, Z. Phys. **223**, 277 (1969).

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

[15]H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1044 (1980).

[16]Technically, the renormalization-group transformation (RGT) can be defined to be $H_{N+2}=R(H_N)$ to avoid the alternation between the energy structures of the Hamiltonian for even and for odd $N$ [See Wilson (Ref. 10) for details.] The RGT has two obvious fixed points corresponding to $\tilde{J}=0$ (free fixed point) and $\tilde{J}=-\infty$ (strong-coupling fixed point). At a fixed point, the many-particle energy levels and matrix elements of

operators are invariant under $R$. For $\tilde{J}=0$, $H_N$ is a quadratic (free-electron) Hamiltonian with $N+1$ operators $(f_0^\dagger, \ldots, f_N^\dagger)$ and can be diagonalized. This leads to two invariant energy-level structures, one for even $N$ and another for odd $N$. For $\tilde{J}=-\infty$, the state created by $f_0^\dagger$ is frozen out since the term $-\Lambda^{(N-1)/2}\tilde{J} f_0^\dagger \boldsymbol{\sigma} f_0 \cdot \mathbf{S}$ must be a singlet for large $|\tilde{J}|$. Thus, $H_N$ is a quadratic form with only $N$ operators $(f_1^\dagger, \ldots, f_N^\dagger)$, and the two fixed points are identical except that the even- and odd-$N$ energy-level structures are interchanged.

[17]C. Jayaprakash, H. R. Krishna-murthy, and J. W. Wilkins, Phys. Rev. Lett. **47**, 737 (1981).
[18]W. Pollwein, T. Höhn, and J. Keller, Z. Phys. B **73**, 219 (1988).
[19]H. Keiter, Z. Phys. **223**, 289 (1969).
[20]V. Zlatić and G. Grüner, J. Phys. (Paris) Lett. **38**, L87 (1977).
[21]F. Mezei and G. Grüner, Phys. Rev. Lett. **29**, 1465 (1972).
[23]J. R. Schrieffer, J. Appl. Phys. **38**, 1143 (1967).