Renormalized parameters and perturbation theory for an *n*-channel Anderson model with Hund's rule coupling: Symmetric case

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We extend the renormalized perturbation theory for the single-impurity Anderson model to the *n*-channel model with a Hund's rule coupling, and show that the exact results for the spin, orbital, and charge susceptibilities, as well as the leading low-temperature dependence for the resistivity, are obtained by working to second order in the renormalized couplings. A universal relation is obtained between the renormalized parameters, independent of *n*, in the Kondo regime. An expression for the dynamic spin susceptibility is also derived by taking into account repeated quasiparticle scattering, which is asymptotically exact in the low-frequency regime and satisfies the Korringa-Shiba relation. The renormalized parameters, including the renormalized Hund's rule coupling, are deduced from numerical renormalization-group calculations for the model for the case $n=2$. The results confirm explicitly the universal relations between the parameters in the Kondo regime. Using these results, we evaluate the spin, orbital, and charge susceptibilities, temperature dependence of the low-temperature resistivity, and dynamic spin susceptibility for the particle-hole symmetric regime of the $n=2$ model.

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I. INTRODUCTION

The single-impurity Anderson model[1] has played an important role in understanding many aspects of the behavior of electrons in systems with strong electron correlation. Nonperturbative methods have had to be developed to make predictions for the behavior of the model in the strong interaction regime. Among the most successful have been the seminal and pioneering work of Wilson and associates[2,3] based on the numerical renormalization group (NRG), and the exact solutions using the Bethe ansatz for the linear dispersion version of the model.[4,5] Though the model was originally put forward to describe magnetic impurities in a host metal, it has proved to be applicable to many other situations. One main area of application is as a model for strong correlation effects in quantum dots.[6] In this application certain parameters of the model, such as the impurity level which determines the electron occupancy on the quantum dot, can be varied by a gate voltage. This makes it possible to sweep through different parameter regimes of the model, which would be difficult to do for real magnetic impurities, and so the predictions of the model can be tested more rigorously. The presence of the narrow many-body resonance in the strong correlation (Kondo) regime at low temperatures can be inferred directly from the measurements of the current through the dot as a function of an applied bias voltage.[7,8]

Apart from these direct applications of the model, it has also played a role in the calculations of strong correlation effects in lattice models. It is possible to map a class of infinite dimensional lattice models of strong electron correlation onto an effective Anderson impurity model with a self-consistency condition, which determines the density of states of the effective medium.[9] This mapping requires that the self-energy is a function of frequency only which is the case in the limit of infinite dimensionality, and the mapping is exact in this limit. For many strongly correlated systems it is known that the wave-vector dependence of the self-energy is much less important than the frequency dependence so this approach can be used as a good first approximation for systems in three dimensions [dynamical mean-field theory (DMFT)]. As the assumption of linear dispersion is not valid for the effective impurity model generated in this application, there are no exact Bethe ansatz solutions so the most reliable nonperturbative approaches, such as the NRG, have to be used.

It has not proved possible so far to access the strong correlation regime of the Anderson model by an approach based purely on perturbation theory in powers of the local interaction U. However, it has been shown that, if the perturbation theory is reorganized such that the basic parameters of the model are renormalized, then a perturbation theory in the renormalized interaction $\tilde{U}$, taken only to second order gives formally the exact results for the low-temperature properties and low-frequency dynamics, provided counter terms are taken into account to avoid overcounting.[10,11] The renormalized parameters have to be determined but these can be calculated very accurately from an analysis of the low-energy excitations of an NRG calculation on the approach to the low-energy fixed point.[12] So far this approach has only been developed in detail for the nondegenerate one channel model but the approach is one that can be applied to a more general class of models including lattice models. Here we extend the calculations to an *n*-channel impurity Anderson model with the inclusion of a Hund's rule exchange term. The Hamiltonian takes the form,

$$\mathcal{H} = \sum_{m\sigma} \epsilon_{dm\sigma} d^{\dagger}_{m\sigma} d_{m\sigma} + \sum_{k,m\sigma} \epsilon_{km\sigma} c^{\dagger}_{km\sigma} c_{km\sigma} + \sum_{km\sigma} (V_k d^{\dagger}_{m\sigma} c_{km\sigma} + V^{*}_k c^{\dagger}_{km\sigma} d_{m\sigma}) + \mathcal{H}_d \qquad (1)$$

where $d^{\dagger}_{m\sigma}$ and $d_{m\sigma}$ are creation and annihilation operators

for an electron in an impurity state with total angular momentum quantum number l, and z component $m=-l,-l+1,\ldots l$, and spin component $\sigma=\uparrow,\downarrow$. The impurity level in a magnetic field H we take as $\epsilon_{dm\sigma}=\epsilon_d-\mu_B\sigma H-\mu_B mH-\mu$, where $\sigma=1$ ($\uparrow$) and $\sigma=-1$ ($\downarrow$) and μ is the chemical potential, and μ_B the Bohr magneton. The creation and annihilation operators $c^\dagger_{km\sigma}$ and $c_{km\sigma}$ are for partial wave conduction electrons with energy $\epsilon_{km\sigma}$. The hybridization matrix element for impurity levels with the conduction-electron states is V_k. We denote the hybridization width factor by $\Delta_{m\sigma}(\epsilon)=\pi\Sigma_k|V_k|^2\delta(\epsilon-\epsilon_{km\sigma})$, which we can take to be a constant Δ in the wide flat-band limit. The remaining part of the Hamiltonian, $\mathcal{H}_d$ describes the interaction between the electrons in the impurity state, which we take to be of the form,

$$\mathcal{H}_d=\frac{(U-J_H)}{2}\sum_{mm'\sigma\sigma'}d^\dagger_{m\sigma}d^\dagger_{m'\sigma'}d_{m'\sigma'}d_{m\sigma}+\frac{J_H}{2}\sum_{mm'\sigma\sigma'}d^\dagger_{m\sigma}d^\dagger_{m'\sigma'}d_{m\sigma'}d_{m'\sigma}. \quad (2)$$

As well as the direct Coulomb interaction U between the electrons, we include a Hund's rule exchange term J_H between electrons in states with different m values. The sign for the exchange term has been chosen so that $J_H>0$ corresponds to a ferromagnetic interaction. This model can be used to describe transition-metal impurities, such as Fe or Cr, in a metallic host in the absence of spin orbit or crystal-field splittings. We can interpret the model more generally with $\alpha=m+l+1$ as a channel index taking values $\alpha=1,2,\ldots n$, where n is the number of channels. The Hund's rule term tends to align the electrons on the impurity site such that for large U and large J_H the impurity state will correspond to a spin $S=n/2$. The model with $J_H=0$ has also been used to describe capacitively coupled double quantum dots,[13] where the impurity channels correspond to different dots. In that application, however, the interdot interaction U' will in general differ from the intradot interaction U so the case here, with $U'=U$, is a special point with SU($2n$) symmetry when $J_H=0$.

The structure of this paper will be as follows. In the next section, we formulate the renormalized perturbation theory (RPT) for this model in terms of the renormalized parameters, $\tilde{\epsilon}_d$, $\tilde{\Delta}$, $\tilde{U}$, and $\tilde{J}_H$. We then show that the low-temperature behavior, as measured by the charge and spin susceptibilities and the low-temperature contribution to the resistivity, can be obtained exactly from the RPT taken to second order in powers of $\tilde{U}$ and $\tilde{J}_H$. In the localized or Kondo regime we show that $\tilde{\Delta}$, $\tilde{U}$, and $\tilde{J}_H$ can be expressed in terms of a single parameter which we take as the Kondo temperature T_K. This relation is independent of the channel index n and hence applies to all values of n. Though we cannot calculate $\tilde{\Delta}$, $\tilde{U}$, and $\tilde{J}_H$ for the general n model using the NRG we can calculate them for the two channel case $n=2$. We look at this in detail for the case of particle-hole symmetry and confirm the universal relations between the renormalized parameters in the Kondo regime predicted using the RPT.

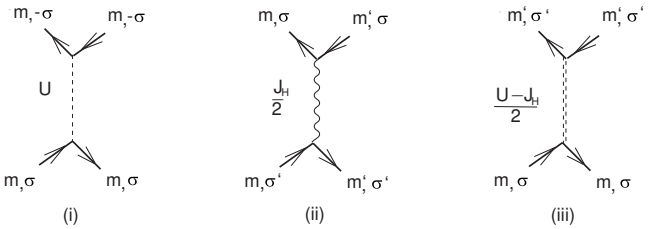

FIG. 1. The three interaction vertices corresponding to the terms in the Hamiltonian given in Eq. (5).

II. RENORMALIZED PERTURBATION THEORY

We start with the Fourier transform of the single-particle Green's function for the impurity d state,

$$G_{d,\sigma}(\omega_{n'})=-\int_0^\beta\langle T_\tau d_{m\sigma}(\tau)d^\dagger_{m\sigma}(0)\rangle e^{i\omega_{n'}\tau}d\tau, \quad (3)$$

where $\omega_{n'}=(2n'+1)/\beta$ and $\beta=1/T$ and the brackets $\langle\ldots\rangle$ denote a thermal average,

$$G_{d,m\sigma}(\omega_n)=\frac{1}{i\omega_n-\epsilon_{dm\sigma}+i\Delta\ \mathrm{sgn}(\omega_n)-\Sigma_{m\sigma}(\omega_n,H)}, \quad (4)$$

where $\Sigma_{m\sigma}(\omega_n,H)$ is the self-energy. For the zero-temperature Green's function, which will be our main concern, ω_n can be replaced by a continuous variable ω, and summations over ω_n replaced by integrations over ω. For the perturbation theory in powers of U and J_H, it will be convenient to separate the interaction terms in the Hamiltonian into the terms involving interactions between electrons in the same channel and those between electrons in different channels. We rewrite the Hamiltonian from Eq. (2) in the form,

$$\mathcal{H}_d=U\sum_m n_{d,m\uparrow}n_{d,m\downarrow}+\frac{(U-J_H)}{2}\sum_{m\neq m'\sigma\sigma'}d^\dagger_{m\sigma}d^\dagger_{m'\sigma'}d_{m'\sigma'}d_{m\sigma}+\frac{J_H}{2}\sum_{m\neq m'\sigma\sigma'}d^\dagger_{m\sigma}d^\dagger_{m'\sigma'}d_{m\sigma'}d_{m'\sigma}. \quad (5)$$

The vertices associated with the three types of interaction terms are illustrated in Fig. 1.

For the renormalized perturbation theory, the Green's function in Eq. (4) can be reexpressed as $G_{d,m\sigma}(\omega_n)=z\tilde{G}_{d,m\sigma}(\omega_n)$, where $\tilde{G}_{d,m\sigma}(\omega_n)$ is the quasiparticle Green's function given by

$$\tilde{G}_{d,m\sigma}(\omega_n)=\frac{1}{i\omega_n-\tilde{\epsilon}_{dm\sigma}+i\tilde{\Delta}\ \mathrm{sgn}(\omega_n)-\tilde{\Sigma}_{m\sigma}(\omega_n,H)} \quad (6)$$

and the renormalized parameters, $\tilde{\epsilon}_{dm\sigma}$ and $\tilde{\Delta}$ are given by

$$\tilde{\epsilon}_{dm\sigma}=z[\epsilon_d+\Sigma_{m\sigma}(0,H)]-\mu_B\sigma H-\mu_B mH,\quad \tilde{\Delta}=z\Delta, \quad (7)$$

where $z=1/[1-\partial\Sigma_{m\sigma}(\omega,0)/\partial(i\omega)]$ evaluated at $\omega=0$. The quasiparticle self-energy $\tilde{\Sigma}_{m,\sigma}(\omega,H)$ is given by

$$\tilde{\Sigma}_{m\sigma}(\omega,H) = z\left(\Sigma_{m\sigma}(\omega,H) - \Sigma_{m\sigma}(0,H) - i\omega \left.\frac{\partial \Sigma_{m\sigma}(\omega,0)}{\partial i\omega}\right|_{\omega=0}\right),$$

where we have assumed the Luttinger theorem,[14] $\mathrm{Im}\,\Sigma(0)=0$, so that $\mathrm{Im}\,\tilde{\Sigma}_{m\sigma}(\omega)\sim\omega^2$ as $\omega\to 0$. When expressed in this form, the $\omega=0$ part of the self-energy and its derivative have been absorbed into renormalizing the parameters $\epsilon_{dm\sigma}$ and Δ, so in setting up the perturbation expansion any further renormalization of these terms must be excluded, or it will result in overcounting. In working with the fully renormalized quasiparticles, it is appropriate to use the renormalized or effective interactions between the quasiparticles. In the single-channel case, we defined the renormalized interaction $\tilde{U}$ in terms of the four vertex $\Gamma_{\uparrow,\downarrow,\downarrow,\uparrow}(\omega_1,\omega_2,\omega_3,\omega_4)$ in the zero-frequency limit.[10] In this case we need to consider the more general four vertex, $\Gamma^{m_1\sigma_1;m_2\sigma_2}_{m_3\sigma_3;m_4\sigma_4}(\omega_1,\omega_2,\omega_3,\omega_4)$, which corresponds to the Fourier coefficient of the connected skeleton diagram for the two-particle Green's function,

$$\langle T_\tau d_{m_1\sigma_1}(\tau_1) d_{m_2\sigma_2}(\tau_2) d^\dagger_{m_3\sigma_3}(\tau_3) d^\dagger_{m_4\sigma_4}(\tau_4)\rangle \tag{8}$$

with the external legs removed. Using the fact that the spin and angular momentum are conserved independently, and taking into account the antisymmetry conditions of the fermion creation and annihilation operators, it was shown by Yoshimori[15] that this vertex at zero frequency can be expressed in terms of two parameters, Γ_C and Γ_e, as

$$\begin{aligned}\Gamma^{m_1\sigma_1;m_2\sigma_2}_{m_3\sigma_3;m_4\sigma_4}(0,0,0,0) = {}& \Gamma_C(\delta^{m_1}_{m_4}\delta^{m_2}_{m_3}\delta^{\sigma_1}_{\sigma_4}\delta^{\sigma_2}_{\sigma_3} - \delta^{m_1}_{m_3}\delta^{m_2}_{m_4}\delta^{\sigma_1}_{\sigma_3}\delta^{\sigma_2}_{\sigma_4}) \\ & + \Gamma_e(\delta^{m_1}_{m_3}\delta^{m_2}_{m_4}\delta^{\sigma_1}_{\sigma_4}\delta^{\sigma_2}_{\sigma_3} - \delta^{m_1}_{m_4}\delta^{m_2}_{m_3}\delta^{\sigma_1}_{\sigma_3}\delta^{\sigma_2}_{\sigma_4}).\end{aligned} \tag{9}$$

To first order in the interaction terms, U and J_{H}, we have $\Gamma_C = U - J_{\mathrm{H}}$ and $\Gamma_e = J_{\mathrm{H}}$. We generalize this result to specify the renormalized parameters, $\tilde{U}$, and $\tilde{J}_{\mathrm{H}}$, by the relation,

$$\begin{aligned}z^2\Gamma^{m_1\sigma_1;m_2\sigma_2}_{m_3\sigma_3;m_4\sigma_4}(0,0,0,0) = {}& (\tilde{U}-\tilde{J}_{\mathrm{H}})(\delta^{m_1}_{m_4}\delta^{m_2}_{m_3}\delta^{\sigma_1}_{\sigma_4}\delta^{\sigma_2}_{\sigma_3} \\ & - \delta^{m_1}_{m_3}\delta^{m_2}_{m_4}\delta^{\sigma_1}_{\sigma_3}\delta^{\sigma_2}_{\sigma_4}) + \tilde{J}_{\mathrm{H}}(\delta^{m_1}_{m_3}\delta^{m_2}_{m_4}\delta^{\sigma_1}_{\sigma_4}\delta^{\sigma_2}_{\sigma_3} \\ & - \delta^{m_1}_{m_4}\delta^{m_2}_{m_3}\delta^{\sigma_1}_{\sigma_3}\delta^{\sigma_2}_{\sigma_4}),\end{aligned} \tag{10}$$

where the factor z^2 arises from the rescaling of the fields to define the quasiparticle Green's function given in Eq. (6). For $n=1$, this reduces to

$$z^2\Gamma^{\sigma_1;\sigma_2}_{\sigma_3;\sigma_4}(0,0,0,0) = \tilde{U}(\delta^{\sigma_1}_{\sigma_4}\delta^{\sigma_2}_{\sigma_3} - \delta^{\sigma_1}_{\sigma_3}\delta^{\sigma_2}_{\sigma_4}), \tag{11}$$

which is the definition of $\tilde{U}$ used in earlier work.[10]

We can combine these terms to define a quasiparticle Hamiltonian $\tilde{H}$,

$$\begin{aligned}\tilde{H} = {}& \sum_{m\sigma}\tilde{\epsilon}_{dm\sigma}\tilde{d}^\dagger_{m\sigma}\tilde{d}_{m\sigma} + \sum_{km\sigma}\epsilon_{km\sigma}c^\dagger_{km\sigma}c_{km\sigma} \\ & + \sum_{km\sigma}(\tilde{V}_k\tilde{d}^\dagger_{m\sigma}c_{km\sigma} + \tilde{V}^*_k c^\dagger_{km\sigma}\tilde{d}_{m\sigma}) + \tilde{H}_d,\end{aligned} \tag{12}$$

$$\begin{aligned}\tilde{H}_d = {}& \frac{(\tilde{U}-\tilde{J}_{\mathrm{H}})}{2}\sum_{mm'\sigma\sigma'} :\tilde{d}^\dagger_{m\sigma}\tilde{d}^\dagger_{m'\sigma'}\tilde{d}_{m'\sigma'}\tilde{d}_{m\sigma}: \\ & + \frac{\tilde{J}_{\mathrm{H}}}{2}\sum_{mm'\sigma\sigma'} :\tilde{d}^\dagger_{m\sigma}\tilde{d}^\dagger_{m'\sigma'}\tilde{d}_{m\sigma'}\tilde{d}_{m'\sigma}:.\end{aligned} \tag{13}$$

The brackets: $\hat{O}$: indicate that the operator $\hat{O}$ within the brackets must be normal ordered with respect to the ground state of the interacting system, which plays the role of the vacuum. This is because the interaction terms only come into play when more than one quasiparticle is created from the vacuum.

The renormalized Hamiltonian is not equivalent to the original model, and the relation between the original and renormalized model is best expressed in the Lagrangian formulation, where frequency enters explicitly.[11] For simplicity, we consider the case in the absence of a magnetic field, where the energy levels $\epsilon_{dm\sigma}$ are independent of m and σ. If the Lagrangian density $\mathcal{L}(\epsilon_d,\Delta,U,J_{\mathrm{H}})$ describes the original model, then by suitably rearranging the terms we can write

$$\mathcal{L}(\epsilon_d,\Delta,U,J_{\mathrm{H}}) = \mathcal{L}(\tilde{\epsilon}_d,\tilde{\Delta},\tilde{U},\tilde{J}_{\mathrm{H}}) + \mathcal{L}_c(\lambda_1,\lambda_2,\lambda_3,\lambda_4), \tag{14}$$

where the remainder part $\mathcal{L}_c(\lambda_1,\lambda_2,\lambda_3,\lambda_4)$ is known as the counter term and takes the form,

$$\begin{aligned}\mathcal{L}_c(\lambda_1,\lambda_2,\lambda_3,\lambda_4) = {}& \sum_{m\sigma}\bar{\tilde{d}}_{m\sigma}(\tau)(\lambda_2\partial_\tau - \lambda_1)\tilde{d}_{m\sigma}(\tau) + (\lambda_3-\lambda_4) \\ & \times \sum_{mm'\sigma\sigma'}\bar{\tilde{d}}_{m,\sigma}(\tau)\bar{\tilde{d}}_{m'\sigma'}(\tau)\tilde{d}_{m'\sigma'}(\tau)\tilde{d}_{m\sigma}(\tau) \\ & + \lambda_4\sum_{mm'\sigma\sigma'}\bar{\tilde{d}}_{m\sigma}(\tau)\bar{\tilde{d}}_{m'\sigma'}(\tau)\tilde{d}_{m,\sigma'}(\tau)\tilde{d}_{m'\sigma}(\tau),\end{aligned} \tag{15}$$

where $\lambda_1=-\Sigma(0)$, $\lambda_2=z-1$, $\lambda_3=(z^2U-\tilde{U})/2$, and $\lambda_4=(\tilde{J}_{\mathrm{H}}-z^2J_{\mathrm{H}})/2$ and $\bar{\tilde{d}}_{m\sigma}(\tau)$, $\tilde{d}_{m\sigma}(\tau)$ are the Grassmann variables corresponding to the d-electron creation and annihilation operators that have to be integrated over in calculating the partition function. Though we can express the coefficients λ_i, $i=1,2,3,4$, explicitly in terms of the self-energy terms and vertices at zero frequency, these relations are not useful in carrying out the expansion. We want to work entirely with the renormalized parameters and carry out the expansion in powers of $\tilde{U}$ and $\tilde{J}_{\mathrm{H}}$. We assume that the λ_i can be expressed in powers of $\tilde{U}$ and $\tilde{J}_{\mathrm{H}}$, and determine them order by order from the conditions that there should be no further renormalization of quantities taken to be already fully renormalized. These conditions are

$$\tilde{\Sigma}_{m\sigma}(0,0) = 0, \qquad \left.\frac{\partial\tilde{\Sigma}_{m\sigma}(\omega,0)}{\partial i\omega}\right|_0 = 0, \tag{16}$$

and that the renormalized four vertex at zero frequency, $\tilde{\Gamma}^{m_1\sigma_1;m_2\sigma_2}_{m_3\sigma_3;m_4\sigma_4}(0,0,0,0)$ is such that

$$\tilde{\Gamma}^{m_1\sigma_1;m_2\sigma_2}_{m_3\sigma_3;m_4\sigma_4}(0,0,0,0) = (\tilde{U}-\tilde{J}_{\rm H})(\delta^{m_1}_{m_4}\delta^{m_2}_{m_3}\delta^{\sigma_1}_{\sigma_4}\delta^{\sigma_2}_{\sigma_3} - \delta^{m_1}_{m_3}\delta^{m_2}_{m_4}\delta^{\sigma_1}_{\sigma_3}\delta^{\sigma_2}_{\sigma_4}) + \tilde{J}_{\rm H}(\delta^{m_1}_{m_3}\delta^{m_2}_{m_4}\delta^{\sigma_1}_{\sigma_4}\delta^{\sigma_2}_{\sigma_3} - \delta^{m_1}_{m_4}\delta^{m_2}_{m_3}\delta^{\sigma_1}_{\sigma_3}\delta^{\sigma_2}_{\sigma_4}). \tag{17}$$

In the field theory context, these conditions are more commonly known as the renormalization conditions. They follow directly from the definitions of the renormalized self-energy in Eq. (7) and the definitions of the renormalized parameters given in Eq. (10).

The propagator in the RPT is the free quasiparticle Green's function,

$$\tilde{G}^{(0)}_{d,m\sigma}(\omega_n) = \frac{1}{i\omega_n - \tilde{\epsilon}_{dm\sigma} + i\tilde{\Delta}\,\mathrm{sgn}(\omega_n)}. \tag{18}$$

The spectral density of the corresponding retarded Green's function gives the free quasiparticle density of states, $\tilde{\rho}^{(0)}_{m\sigma}(\omega)$ given by

$$\tilde{\rho}^{(0)}_{m\sigma}(\omega) = \frac{\tilde{\Delta}/\pi}{(\omega-\tilde{\epsilon}_{dm\sigma})^2 + \tilde{\Delta}^2}. \tag{19}$$

From Fermi-liquid theory, the quasiparticle interaction terms do not contribute to the linear specific-heat coefficient γ of the electrons. It follows that the impurity contribution to this coefficient is proportional to the free quasiparticle density of states evaluated at the Fermi level and is given by

$$\gamma = \frac{\pi^2}{3}\sum_{m,\sigma}\tilde{\rho}^{(0)}_{m\sigma}(0). \tag{20}$$

In the absence of a magnetic field, this reduces to $\gamma = 2n\pi^2\tilde{\rho}^{0}(0)/3$, where $\tilde{\rho}^{(0)}(0)$ is the quasiparticle density of states per single spin and channel.

If we integrate the free quasiparticle density of states in Eq. (19) to the Fermi level then we get $\langle\tilde{n}_{dm\sigma}\rangle$ at $T=0$, which is given by

$$\langle\tilde{n}_{dm\sigma}\rangle = \frac{\eta_{m\sigma}}{\pi} = \frac{1}{2} - \frac{1}{\pi}\tan^{-1}\left(\frac{\tilde{\epsilon}_{dm\sigma}}{\tilde{\Delta}}\right), \tag{21}$$

which defines the phase shift $\eta_{m\sigma}$ in the channel with quantum numbers m and σ. For this model, it has been shown by Shiba[16] that $\langle n_{dm\sigma}\rangle = \eta_{m\sigma}/\pi$, giving a generalization of the Friedel sum rule, so that we have $\langle\tilde{n}_{dm\sigma}\rangle = \langle n_{dm\sigma}\rangle$; the quasiparticle occupation number in each channel is equal to the impurity occupation number in that channel. However, Yoshimori and Zawadowski[17] have shown that this form of the Friedel sum rule does not hold for a more general model in which scattering processes can occur between m states, $m_1, m_2 \to m_3, m_4$, such that $m_1+m_2=m_3+m_4$. They derive a restricted form of the sum rule such that $\Sigma_{m\sigma}a_{m\sigma}\langle\tilde{n}_{dm\sigma}\rangle = \Sigma_{m\sigma}a_{m\sigma}\eta_{dm\sigma}/\pi$, where $a_{m\sigma}=1,\sigma,m$. In this more general case, therefore, the quasiparticle number does not equal the occupation number in the same channel but we have the more restricted result, $\Sigma_{m\sigma}a_{m\sigma}\langle\tilde{n}_{dm\sigma}\rangle = \Sigma_{m\sigma}a_{m\sigma}\langle n_{dm\sigma}\rangle$. Using either result, however, we can derive expressions for the zero-field spin χ_s, orbital χ_{orb}, and charge χ_c susceptibilities. We differentiate the combinations, $\Sigma_{m\sigma}a_{m\sigma}\langle\tilde{n}_{d,m\sigma}\rangle$, with $a_{m\sigma} = \sigma$, m and 1, respectively, with respect to the magnetic field or in the charge case with respect to ϵ_d. To evaluate these expressions we need to calculate the renormalized self-energy. This calculation taken to first order in $\tilde{U}$ and $\tilde{J}_{\rm H}$ proceeds as in the one-channel case,[10,11] and gives

$$\chi_s = 2n\mu_{\rm B}^2\tilde{\rho}^{(0)}(0)\{1+[\tilde{U}+(n-1)\tilde{J}_{\rm H}]\tilde{\rho}^{(0)}(0)\}, \tag{22}$$

$$\chi_{orb} = \frac{(n^2-1)\mu_{\rm B}^2\tilde{\rho}^{(0)}(0)}{12}[1+(\tilde{U}-3\tilde{J}_{\rm H})\tilde{\rho}^{(0)}(0)], \tag{23}$$

and

$$\chi_c = 2n\tilde{\rho}^{(0)}(0)\{1-[(2n-1)\tilde{U}-3(n-1)\tilde{J}_{\rm H}]\tilde{\rho}^{(0)}(0)\}. \tag{24}$$

These results can also be obtained from a mean-field theory on the quasiparticle part of the Hamiltonian given in Eq. (13).[18,19] It can be shown using the Ward identities derived by Yoshimori,[15] which are generalizations of the Ward identities derived by Yamada[20,21] for the single-channel case, that these results are exact. Hence all higher-order correction terms in $\tilde{U}$ and $\tilde{J}_{\rm H}$ cancel out.

In the localized regime a large value of U suppresses the charge fluctuations on the impurity so $\chi_c \sim 0$. Treating this as an equality, we get a relation between $\tilde{\rho}^{(0)}(0)$, $\tilde{U}$, and $\tilde{J}_{\rm H}$,

$$[(2n-1)\tilde{U}-3(n-1)\tilde{J}_{\rm H}]\tilde{\rho}^{(0)}(0) = 1. \tag{25}$$

Similarly when the Hund's rule interaction $J_{\rm H}$ (>0) is large it will suppress the local orbital fluctuations, as the configuration with the spins aligned will be favored. For $J_{\rm H} \gg \pi\Delta$, we can expect the orbital fluctuations to be almost fully suppressed so that $\chi_{orb} \sim 0$ which, as an equality, gives a further relation between $\tilde{\rho}^{(0)}(0)$, $\tilde{U}$, and $\tilde{J}_{\rm H}$,

$$(3\tilde{J}_{\rm H}-\tilde{U})\tilde{\rho}^{(0)}(0) = 1. \tag{26}$$

We explore the consequences of the relation (26) first of all for the model with $J_{\rm H}=0$. If we combine the orbital m and spin indices σ into an index $\nu=(m,\sigma)$ then it can be shown that the model with $J_{\rm H}=0$ has SU($2n$) symmetry so we will refer to the model in this limit as the SU($2n$) Anderson model.[22] With $J_{\rm H}=0$, in the localized limit we have from Eq. (25),

$$\tilde{U} = \frac{\pi\tilde{\Delta}}{(2n-1)}, \tag{27}$$

which agrees with the one channel result $\tilde{U}=\pi\tilde{\Delta}$ for $n=1$. This gives a "χ/γ" or Wilson ratio, $R_{\rm W} = \pi^2\chi_s/3\mu_{\rm B}^2\gamma = 2n/(2n-1)$.

We return to consider the model with a finite Hund's rule coupling $J_{\rm H} \neq 0$. For the case of half filling, where $\tilde{\epsilon}_d=0$ and $\tilde{\rho}^{(0)}(0)=1/\pi\tilde{\Delta}$, the nonlinear relation between the renormalized parameters in Eqs. (25) and (26) become linear relations between $\tilde{\Delta}$, $\tilde{U}$, and $\tilde{J}_{\rm H}$,

$$\pi\tilde{\Delta} = (2n-1)\tilde{U} - 3(n-1)\tilde{J}_{\mathrm{H}} \tag{28}$$

and

$$\pi\tilde{\Delta} = 3\tilde{J}_{\mathrm{H}} - \tilde{U}. \tag{29}$$

An equivalent condition to that in Eq. (29) can be obtained using the argument of Nozières and Blandin[23] that the occupation number in a channel m should be independent of any small change in the chemical potential in a channel $m' \neq m$ in this regime. When both the local charge and orbital fluctuations are suppressed, the renormalized parameters can be expressed in terms of the Kondo temperature T_{K}. We define T_{K} by writing the spin susceptibility in the form,

$$\chi_s = \frac{(g\mu_{\mathrm{B}})^2 S(S+1)}{3T_{\mathrm{K}}}, \tag{30}$$

where $S=n/2$ and $g=2$. From Eq. (22) we deduce that $1/\tilde{\rho}^{(0)}(0)=4T_{\mathrm{K}}$, which gives for the Wilson ratio in the Kondo limit, $R_{\mathrm{W}}=\pi^2\chi_s/3\mu_{\mathrm{B}}^2\gamma=2(n+2)/3$.[15,23]

From Eqs. (25) and (26) for the particle-hole symmetric case, we find $1/\tilde{\rho}^{(0)}(0)=\pi\tilde{\Delta}=4T_{\mathrm{K}}$, and we then find

$$\pi\tilde{\Delta} = \tilde{U} = \frac{3}{2}\tilde{J}_{\mathrm{H}} = 4T_{\mathrm{K}}, \tag{31}$$

which was conjectured earlier on the basis of a phenomenological mean-field approach.[18,19] A notable feature of this result is that there is no explicit dependence on n.

Yoshimori[15] has also derived an exact result for the low-temperature impurity contribution to the resistivity in the particle-hole symmetric case and $H=0$. In terms of the renormalized parameters, the result is

$$R(T) = R_0\left[1 - \frac{\pi^4(1+2I_R)T^2}{3} + \mathrm{O}(T^4)\right], \tag{32}$$

where I_R is given by

$$I_R = [\tilde{\rho}^{(0)}(0)]^2[(2n-1)\tilde{U}^2 - 6(n-1)\tilde{J}_{\mathrm{H}}(\tilde{U}-\tilde{J}_{\mathrm{H}})]. \tag{33}$$

This result can be derived in the RPT from a calculation of the renormalized self-energy $\tilde{\Sigma}(\omega)$ to second order in $\tilde{U}$ and $\tilde{J}_{\mathrm{H}}$. With the Hund's rule interaction term, there are several types of second-order scattering diagrams which are illustrated in Fig. 2. The vertices are of the same type as shown in Fig. 1 but are weighted by the renormalized interaction terms. The calculations follow along similar lines to those for the single-channel case $n=1$.[10,11] The first-order diagrams and the terms linear in ω are canceled by the counter terms to this order, and there are no corrections from the counter terms to the vertices to second order for the case with particle-hole symmetry. The contributions to I_R from diagrams of the types (i) to (iv), respectively, in units of $[\tilde{\rho}^{(0)}(0)]^2$ are $\tilde{U}^2$; $2(n-1)\tilde{J}_{\mathrm{H}}^2$; $2(n-1)(\tilde{U}-\tilde{J}_{\mathrm{H}})^2$; $-2(n-1)\tilde{J}_{\mathrm{H}}(\tilde{U}-\tilde{J}_{\mathrm{H}})$; which give the result in Eq. (33).

In the localized regime at half filling the result in Eq. (32) simplifies to give

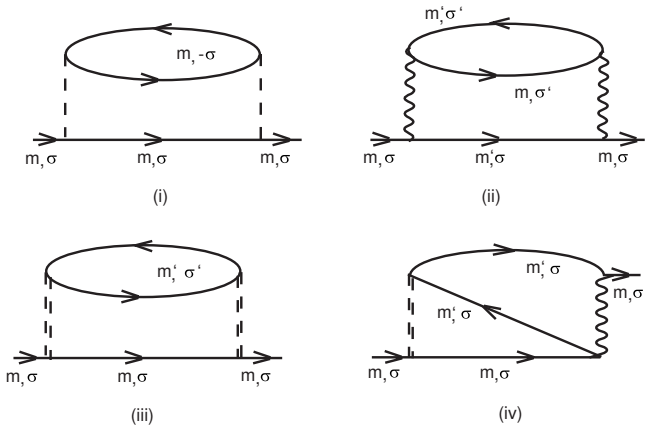

FIG. 2. Second-order diagrams in the renormalized perturbation theory.

$$R(T) = R_0\left[1 - \frac{\pi^4(5+4n)}{96}\left(\frac{T}{T_{\mathrm{K}}}\right)^2 + \mathrm{O}(T^4)\right], \tag{34}$$

which agrees with the result derived by Nozières[24] and Yamada[20,21] for the case $n=1$. Thus all the exact Fermi-liquid relations can be derived from the RPT taken to second order only.

It was shown in earlier work[25] that the RPT approach can provide a description of the dynamic spin susceptibility for the $n=1$ model in the low-frequency regime. The calculation takes account of the repeated quasiparticle scattering, giving results which are exact in the low-frequency limit $\omega \to 0$, and in remarkably good agreement with the results from a direct NRG calculation. We extend the calculation to the n-channel model given in Eqs. (1) and (2). We consider the Fourier transform of the transverse spin susceptibility,

$$\chi_s^{+-}(i\omega_{n'}) = \int_0^\beta \left\langle T_\tau \sum_m S_{d,m}^+(\tau) \sum_{m'} S_{d,m'}^-(0) \right\rangle e^{i\omega_{n'}\tau} d\tau, \tag{35}$$

where $\omega_{n'}=2\pi n'/\beta$ and $S_{d,m}^+ = d_{m\uparrow}^\dagger d_{m\downarrow}$, $S_{d,m}^- = d_{m\downarrow}^\dagger d_{m\uparrow}$ $[S_{d,m}^z = (n_{d,\uparrow}-n_{d,\downarrow})/2]$. We consider the scattering of a spin-up quasiparticle with a spin-down quasihole both in channel m, in the absence of a magnetic field. This particle-hole pair can scatter into a particle-hole pair in the same channel m or a different channel $m' \neq m$. We consider the scattering into the same channel first of all. The matrix element for this process is $\tilde{U}$, except we must allow for the fact that $\tilde{U}$ already takes into account these processes for $\omega=0$ so, to prevent overcounting, we must use $\tilde{U}-\lambda_3$, where λ_3 is the corresponding counter term. It will be convenient to use the notation $\tilde{U}_{\mathrm{eff}}$ for $\tilde{U}-\lambda_3$. Just taking this type of repeated scattering into account gives us a result which has the same form as in the single-channel case $n=1$,[25]

$$\chi_s^{+-}(\omega+i\delta) = 4n\mu_{\mathrm{B}}^2 \frac{\tilde{\Pi}^{+-}(\omega+i\delta)}{1-\tilde{U}_{\mathrm{eff}}\tilde{\Pi}^{+-}(\omega+i\delta)}, \tag{36}$$

where we have analytically continued to real frequency ω. The free quasiparticle-quasihole propagator in a single chan-

nel, $\tilde{\Pi}^{+-}(\omega+i\delta)$, is independent of the channel index in the absence of a magnetic field, and is given by

$$\tilde{\Pi}^{+-}(\omega+i\delta)=\frac{\tilde{\Delta}}{\pi(\tilde{\epsilon}_d^2+\tilde{\Delta}^2)}, \quad \omega=0$$

$$=\frac{-\tilde{\Delta}}{\pi\omega(\omega+2i\tilde{\Delta})}\left\{\ln\left(1+\frac{\omega}{\tilde{\epsilon}_d+i\tilde{\Delta}}\right)+\ln\left(1-\frac{\omega}{\tilde{\epsilon}_d-i\tilde{\Delta}}\right)\right\} \quad \omega\neq 0 \tag{37}$$

for $\delta\to+0$. We must also take into account that the quasiparticle-quasihole pair being created in channel m can scatter into a different channel m', and also be finally annihilated in a channel with $m'\neq m$. The matrix element for this type of scattering is $\tilde{J}_{\mathrm{H}}$, corresponding to the diagram in Fig. 1 (ii), but again, to avoid overcounting, we replace it by $\tilde{J}_{\mathrm{H}}^{\mathrm{eff}}$. In the absence of a magnetic field, the quasiparticle-quasihole propagator is independent of the channel index m, so the summation over the states m' introduces a factor $n-1$. The result of taking these scattering processes into account is that the pair propagator $\tilde{\Pi}^{+-}(\omega+i\delta)$ in Eq. (36) is replaced by

$$\frac{\tilde{\Pi}^{+-}(\omega+i\delta)}{1-\tilde{J}_H^{\mathrm{eff}}(n-1)\tilde{\Pi}^{+-}(\omega+i\delta)}, \tag{38}$$

which leads to the result,

$$\chi_s^{+-}(\omega+i\delta)=4n\mu_{\mathrm{B}}^2\frac{\tilde{\Pi}^{+-}(\omega+i\delta)}{1-[\tilde{U}_{\mathrm{eff}}+(n-1)\tilde{J}_H^{\mathrm{eff}}]\tilde{\Pi}^{+-}(\omega+i\delta)}. \tag{39}$$

We need to determine the combination $\tilde{U}_{\mathrm{eff}}+(n-1)\tilde{J}_{\mathrm{H}}^{\mathrm{eff}}$. We can do this by requiring that this expression gives $2\chi_s$ in the zero-frequency limit, which is equivalent to the requirement that these scattering processes contribute to the four vertex at zero frequency are not overcounted. This condition gives

$$\tilde{U}_{\mathrm{eff}}+(n-1)\tilde{J}_H^{\mathrm{eff}}=\frac{\tilde{U}+(n-1)\tilde{J}_H}{1+[\tilde{U}+(n-1)\tilde{J}_H]\tilde{\rho}^{(0)}(0)}. \tag{40}$$

In the Kondo regime, this condition simplifies to $\tilde{U}_{\mathrm{eff}}+(n-1)\tilde{J}_H^{\mathrm{eff}}=2T_{\mathrm{K}}(1+2n)/(2+n)$, which gives the one-channel result $\tilde{U}_{\mathrm{eff}}=2T_{\mathrm{K}}$ for $n=1$.

By rewriting Eq. (39) in the form,

$$\frac{4n\mu_{\mathrm{B}}^2}{\chi_s^{+-}(\omega+i\delta)}=\frac{1}{\tilde{\Pi}^{+-}(\omega+i\delta)}-[\tilde{U}_{\mathrm{eff}}+(n-1)\tilde{J}_H^{\mathrm{eff}}], \tag{41}$$

and taking the imaginary part, it is straight forward to show that the expression for $\chi_s(\omega)$ satisfies the exact Korringa-Shiba relation,

$$\lim_{\omega\to 0}\frac{\mathrm{Im}\,\chi^{+-}(\omega+i\delta)}{\omega}=\frac{\pi\chi_s^2}{n\mu_{\mathrm{B}}^2}, \tag{42}$$

which was proved for this model by Shiba[16] and more generally by Yoshimori and Zawadowsi.[17]

So far we have not discussed how one can calculate the renormalized parameters $\tilde{\epsilon}_d$, $\tilde{\Delta}$, $\tilde{U}$, and $\tilde{J}_{\mathrm{H}}$. In the Kondo regime, these reduce to a single parameter T_{K} so one possibility is to deduce its value from experiment by fitting the predictions to the measurements of a physical quantity in the low-temperature regime, say, the impurity susceptibility or resistivity. Outside the Kondo regime, we have four parameters to determine, and to calculate all four from experiment one loses much of the predictive power of the approach. However, it was shown earlier for the single-channel Anderson model how the parameters, $\tilde{\epsilon}_d$, $\tilde{\Delta}$, and $\tilde{U}$, can be calculated in terms of the bare parameters, ϵ_d, Δ, and U, from the many-body low-energy excitations of an NRG calculation.[12] There are problems in carrying out this procedure for the general n-channel model, due to the truncation of states which has to be carried out in an NRG calculation to reach the very low-energy scales. Truncation means that only a fraction $1/4^n$ states can be retained at each NRG iteration. It is possible, however, for the case $n=2$ to compensate for the lower percentage by increasing the number of states kept at each iteration as the matrices do not get so large. In the next section, we present calculations of $\tilde{\Delta}$, $\tilde{U}$, and $\tilde{J}_{\mathrm{H}}$, in terms of Δ, U, and J_{H}, for the $n=2$ model.

III. NRG CALCULATION OF THE RENORMALIZED PARAMETERS FOR N=2

The two-channel model the Hamiltonian $\mathcal{H}_d$ given in Eq. (2) can be reexpressed in the form,

$$\mathcal{H}_d=U\sum_{\alpha=1,2}n_{d\alpha\uparrow}n_{d\alpha\downarrow}+U_{12}\sum_{\sigma\sigma'}n_{d,1\sigma}n_{d,2\sigma'}-2J_{\mathrm{H}}\mathbf{S}_{d,1}\cdot\mathbf{S}_{d,2} \tag{43}$$

with a ferromagnetic Heisenberg exchange coupling $2J_{\mathrm{H}}$ between the electrons in the different channels, and $U_{12}=U-3J_{\mathrm{H}}/2$. Our calculations will be restricted to the particle-hole symmetric model so we take $\epsilon_d=-U/2-U_{12}$ in the one-electron part of the Hamiltonian given in Eq. (1). The energy of the two-electron triplet state of the isolated impurity with particle-hole symmetry is $-2U+J_{\mathrm{H}}$ and that of the four-electron or zero-electron state is 0 so if we are interested in the case when the triplet state is the ground-state configuration, we need to consider the regime $U>J_{\mathrm{H}}/2$.

For the NRG calculations, the model is recast in a form such that the impurity is coupled via a hybridization V to two tight-binding chains which describe the conduction-electron states, one chain for each channel. The conduction-electron band is discretized with a discretization parameter $\Lambda>1$, such that the couplings decrease along the chains as $\Lambda^{-N/2}$ for large N, where N is the Nth site along the chain from the impurity. The calculations are then carried out iteratively by direct diagonalization, starting at the impurity site and adding one further site to each chain at each iteration step. The

number of basis states used has to be truncated when the matrices get too large for diagonalization on a practical time scale, which can occur after only a few iterative steps. When truncation is applied a fixed number of states is retained at each step. For the $n=2$ model considered here, we take 3600 states, which is a factor of 3 to 4 more than for the nondegenerate model ($n=1$) and a discretization factor $\Lambda=6$. We can check the expected accuracy of our calculations by using this value for Λ to calculate $\tilde{U}$ and $\pi\tilde{\Delta}$ for the single-channel model and compare with the values deduced indirectly from the exact Bethe ansatz results for the specific-heat coefficient γ and the zero-temperature spin susceptibility.[12] For $U/\pi\Delta=2$, $\pi\Delta=0.01$, keeping 900 states, we get the values, $\tilde{U}=0.2295$ and $\pi\tilde{\Delta}=0.2387$, which can be compared with those deduced from the Bethe ansatz, $\tilde{U}=0.2301$ and $\pi\tilde{\Delta}=0.2392$. This gives an accuracy of better than 0.3%. For further details on setting up the NRG calculations, we refer to the original papers[2,3] and the recent review article.[26]

With this discrete spectrum, the Green's function in Eq. (4) takes the form,

$$G_{d,\sigma}(\omega)=\frac{1}{i\omega-\epsilon_{dm\sigma}-|V|^2 g_{\alpha\sigma}(i\omega)-\Sigma_{m\sigma}(\omega)}, \tag{44}$$

where $g_{\alpha\sigma}(i\omega)$ is the Green's function for the first site for the isolated conduction-band chain.

The connection between the NRG approach and the renormalized perturbation theory is based on identifying the quasiparticle Hamiltonian, given in Eqs. (12) and (13), as the low-energy fixed point of the NRG together with the leading irrelevant terms.[27] The lowest single-particle excitations from the NRG ground state should correspond to a quasiparticle excitation described by the one-body part of the quasiparticle Hamiltonian as given in Eq. (12). For the calculation of the interaction terms, $\tilde{U}$ and $\tilde{J}_{\mathrm{H}}$, from the NRG we have to consider the difference between two-body excitations from the NRG ground state and the two corresponding one-body excitations.

The low-energy single-particle excitations are given by the poles of the noninteracting quasiparticle Green's function when analytically continued to real frequency ω. The equation for these poles is the same as that for the noninteracting model but with a renormalized hybridization $\tilde{V}$ and energy level $\tilde{\epsilon}_d$. Therefore, the lowest-energy single-particle and hole excitations, $E_p(N)$ and $E_h(N)$, from the *interacting* ground state should be solutions of the equation,

$$\omega-\tilde{\epsilon}_d-|\tilde{V}|^2 g_{\alpha\sigma}(\omega)=0. \tag{45}$$

If we substitute the excitations energies, $E_p(N)$ and $E_h(N)$, as calculated in the NRG for a finite chain length N, into Eq. (45) then we can deduce corresponding N-dependent renormalized parameters $\tilde{V}(N)$ and $\tilde{\epsilon}_d(N)$. Only if $\tilde{V}(N)$ and $\tilde{\epsilon}_d(N)$ become independent of N for large N, do the low-energy one-particle energy levels of the interacting system correspond to those of a renormalized noninteracting model. If this is the case, then the asymptotic values for large N define the renormalized parameters $\tilde{V}$ (and hence $\tilde{\Delta}$) and $\tilde{\epsilon}_d$.

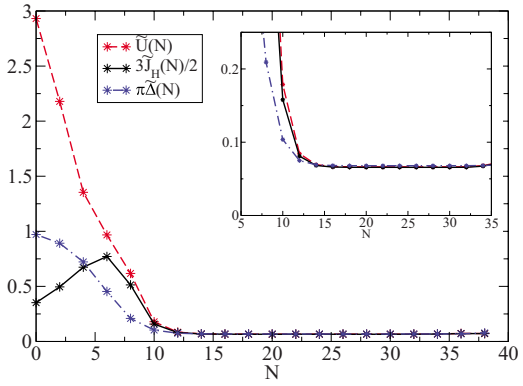

FIG. 3. (Color online) A plot of $\pi\tilde{\Delta}(N)/\pi\Delta$, $\tilde{U}(N)/\pi\Delta$, and $3\tilde{J}_{\mathrm{H}}(N)/2\pi\Delta$ versus N for $U/\pi\Delta=3.6$ $J_{\mathrm{H}}/\pi\Delta=0.15$, and $\pi\Delta=0.01$. The inset shows the convergence of these parameter to a common limit in this case as the bare parameters correspond to a point in the Kondo regime.

To calculate the renormalized interaction terms, we first have to diagonalize the noninteracting impurity model with the renormalized parameters, which describes the quasiparticles. The interaction terms are then added to the quasiparticle Hamiltonian and expressed using the diagonalized single quasiparticle states as a basis. The energy difference between the lowest two-particle state and the sum of the corresponding two quasiparticle states is equal to the expectation value of interaction terms in the quasiparticle Hamiltonian. The interaction parameter $\tilde{U}$ can be calculated from the NRG results for the lowest two-particle excitation in the *same* channel which will be independent of $\tilde{J}_{\mathrm{H}}$. For a finite length chain N, the value $\tilde{U}(N)$ will depend upon N, and for this to correspond to a low-energy quasiparticle Hamiltonian $\tilde{U}(N)$ should become independent of N for large N. The asymptotic values of $\tilde{U}(N)$ for large N defines the renormalized parameter $\tilde{U}$. Similarly, to calculate $\tilde{J}_{\mathrm{H}}$ we look at the difference between the single and triplet states of a two-particle excitation with one electron excitation in each of the two channels. This excitation will be independent of $\tilde{U}$ and depend only on $\tilde{J}_{\mathrm{H}}$. Using the NRG results for a finite chain of N sites, we can define a parameter $\tilde{J}_{\mathrm{H}}(N)$, with $\tilde{J}_{\mathrm{H}}$ given by the asymptotic value of $\tilde{J}_{\mathrm{H}}(N)$ for large N. Further details on the calculations of the renormalized parameters from the low energy NRG states can be found in Ref. 12.

We first show results for the renormalized parameters as a function of N. We show a typical case in Fig. 3 for the parameters $\tilde{U}(N)$, $\pi\tilde{\Delta}(N)$, and $3\tilde{J}_{\mathrm{H}}(N)/2$ as a function of N for $\pi\Delta=0.01$, $U/\pi\Delta=3.6$, and $J_{\mathrm{H}}/\pi\Delta=0.15$, which is a parameter set corresponding to a point in the Kondo regime where the orbital fluctuations have been suppressed. The results demonstrate that not only is there a plateau region for all the parameters for large N but also that the asymptotic values of $\tilde{U}(N)$, $\pi\tilde{\Delta}(N)$, and $3\tilde{J}_{\mathrm{H}}(N)/2$ correspond to a single energy scale and satisfy the relation given in Eq. (31). The choice of a relatively large value of $\Lambda=6$ means that the convergence to a plateau region is achieved for relatively

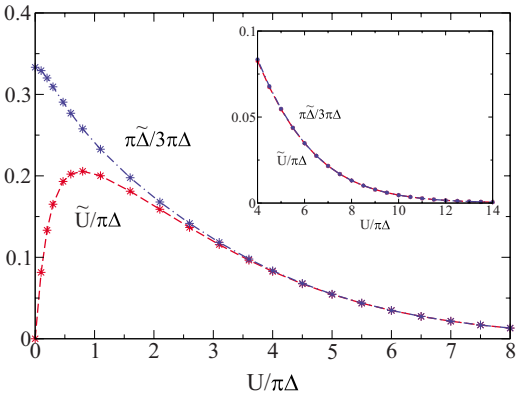

FIG. 4. (Color online) A plot of $\pi\tilde{\Delta}/3\pi\Delta$ and $\tilde{U}/\pi\Delta$ versus $U/\pi\Delta$ for $J_{\mathrm{H}}=0$ and $\pi\Delta=0.01$.

small values of N. The plateau region is finite because the renormalized parameters correspond to the leading irrelevant corrections to the free fermion fixed point of the Wilson renormalization-group transformation[2] so eventually they diverge from the plateau when N is such that the decreasing irrelevant corrections become of the same order as the uncertainties in the numerical computation.

Having described how to calculate the the renormalized parameters and established that the method is capable of providing very accurate results for the model including the Hund's rule coupling, we investigate in detail the results in the different parameter regimes.

A. SU(4) model ($J_{\mathrm{H}}=0$): Symmetric case

We begin with the results for the model with $J_{\mathrm{H}}=0$ which has SU(4) symmetry, and restrict our attention for the moment to the particle-hole symmetric case. In Fig. 4, we show the results for $\tilde{\Delta}/3\Delta$ and $\tilde{U}/\pi\Delta$ versus $U/\pi\Delta$ ($J_{\mathrm{H}}=0$, $\pi\Delta=0.01$). We predicted from Eq. (27) that for large $U/\pi\Delta$ we should have a single energy scale such that for $n=2$, $\tilde{U}=\pi\tilde{\Delta}/3$ and the results clearly show that this is the case for $U/\pi\Delta>3$. The numerical results for the ratio $\tilde{U}/\pi\tilde{\Delta}$ for large U give the value 1/3 to an accuracy of 0.01%.

In Figs. 5 and 6, we compare the results for these two quantities with those for the single-channel model $n=1$. We can see that the parameters $\tilde{\Delta}$ and $\tilde{U}$ the fall off with increase in U much more slowly for the two channel model. This is because in the two-channel model, we have unsuppressed fluctuations of the orbital component. When $J_{\mathrm{H}}=0$ and finite U, at half filling in the isolated impurity for the two-channel model there are six degenerate two-electron configurations with energy $2\epsilon_d+U$. Both the $n=1$ and $n=2$ models in the Kondo regime can be described by localized SU($2n$) Kondo model. For the case $n=1$ it is the s-d or SU(2) Kondo model and for $n=2$ the Coqblin-Schrieffer or SU(4) Kondo model.[32] The Hamiltonian for the SU($2n$) Kondo model takes the form,

$$\mathcal{H}_K(2n)=J_{\mathrm{eff}}\sum_{\nu,\nu',k,k'}Y_{\nu,\nu'}c^{\dagger}_{k',\nu'}c_{k,\nu}+\sum_{\nu,k}\epsilon_k c^{\dagger}_{k,\nu}c_{k,\nu}, \quad (46)$$

where the sum over $\nu=1,2,\ldots 2n$, and with particle-hole symmetry $J_{\mathrm{eff}}=4|V|^2/U$. The operators $Y_{\nu,\nu'}$ obey the SU($2n$) commutation relations,

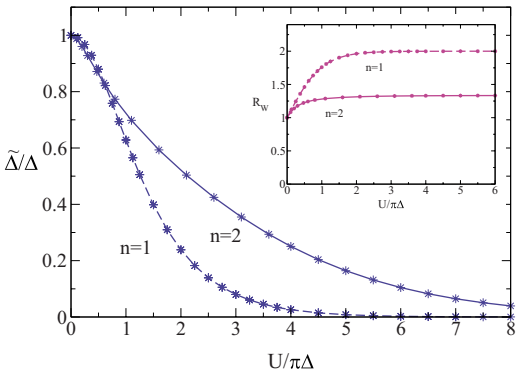

FIG. 5. (Color online) A comparison of $\tilde{\Delta}/\Delta$ versus $U/\pi\Delta$ for the $n=1$ and $n=2$ models for $J_{\mathrm{H}}=0$ and $\pi\Delta=0.01$. The inset shows the corresponding values for the Wilson ratio $R_{\mathrm{W}}=1+\tilde{U}/\pi\tilde{\Delta}$.

$$[Y_{\nu,\nu'},Y_{\nu'',\nu'''}]_-=Y_{\nu,\nu'''}\delta_{\nu',\nu''}-Y_{\nu'',\nu'}\delta_{\nu,\nu'''}, \quad (47)$$

with $\Sigma_\nu Y_{\nu,\nu}=nI$. For $n=1$, $Y_{\nu,\nu'}=|\nu\rangle\langle\nu'|$, where $|\nu\rangle$ are the single-electron impurity states with spin up ($\nu=1$) and spin down ($\nu=2$), giving a two-dimensional representation for the $Y_{\nu,\nu'}$. In the two-channel case for half filling, the representation of the operators $Y_{\nu,\nu'}$ is six dimensional and details of the $Y_{\nu,\nu'}$ in terms of the two-electron impurity states are given in the Appendix.

In the single-channel case $n=1$, T_{K} is known from the Bethe ansatz solution, and is given by $T_{\mathrm{K}}/\pi\Delta=\sqrt{u/2\pi}e^{-\pi^2u/8+0.5/u}$, where $u=U/\pi\Delta$,[28] and the NRG results for T_{K} deduced from $\pi\tilde{\Delta}$ are in precise agreement with this expression for large U. For $n\geq 2$, there is no Bethe ansatz solution for the model with finite U. However, there is a Bethe ansatz solution for the SU(N) Kondo model (Coqblin-Schrieffer model) and the N-fold degenerate Anderson model with $U=\infty$ (Refs. 29–31) which gives in the exponential for T_{K} a factor proportional to $1/N$. The prefactor is not universal and depends on the cutoffs used for the high-energy excitations in the model. We have taken for the two-channel case, therefore, the expression $T_{\mathrm{K}}/\pi\Delta=1.01ue^{-\pi^2u/16+0.25/u}/2\pi$, where the prefactor has been chosen to give the most reasonable fit to the data. The result of this fitting is shown in Fig. 7, where it can been seen that the

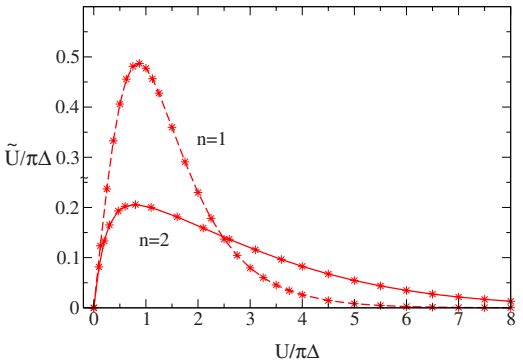

FIG. 6. (Color online) A comparison of $\tilde{U}/\pi\Delta$ versus $U/\pi\Delta$ for the $n=1$ and $n=2$ models for $J_{\mathrm{H}}=0$ and $\pi\Delta=0.01$.

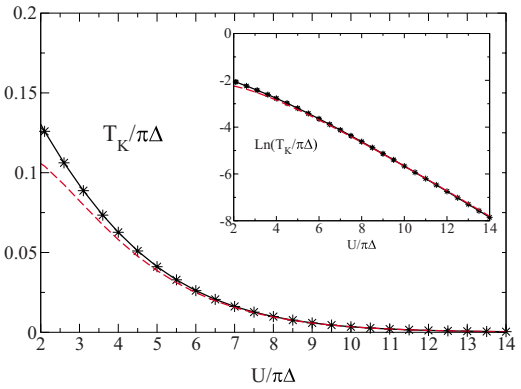

FIG. 7. (Color online) A plot of $T_K/\pi\Delta$ as a function of $U/\pi\Delta$ for $J_H=0$ and $\pi\Delta=0.01$. The dashed curve corresponds to the formula $1.01ue^{-\pi^2u/16+0.25/u}/2\pi$, where $u=U/\pi\Delta$. The inset shows a plot of the logarithm for the same two curves.

agreement is very good in the strong-coupling range $U/\pi\Delta > 4.0$. The same form for T_K was used in Ref. 22, and found to be in good agreement with their NRG results.

B. Model with $J_H \neq 0$: Symmetric case

In Fig. 8, we look at the effect of switching on the Hund's rule term J_H for a relatively large value of U, $U/\pi\Delta=4.0$, which is sufficient to suppress the charge fluctuations. As we increase J_H, we begin to suppress also the orbital fluctuations, such that when $J_H/\pi\Delta > 0.1$ we are in the regime where we have a single energy scale. This we refer to as the Kondo regime with the Kondo temperature in the particle-hole symmetric case given by $\pi\tilde{\Delta}=4T_K$. The Wilson ratio is shown in the inset of Fig. 8 and rises steadily from the value 4/3 for $J_H=0$ to 8/3 in the Kondo regime, corresponding to the results given earlier for these limits, $2n/(2n-1)$ and $2(n+2)/3$, for $n=2$. We note also in the Kondo regime the renormalized parameters are such that $\tilde{U}_{12}=\tilde{U}-3\tilde{J}_H/2=0$.

In Fig. 9, we plot the corresponding spin, orbital, and charge susceptibilities using the expression for these given in Eqs. (22)–(24) for the set of parameters used for Fig. 8. The

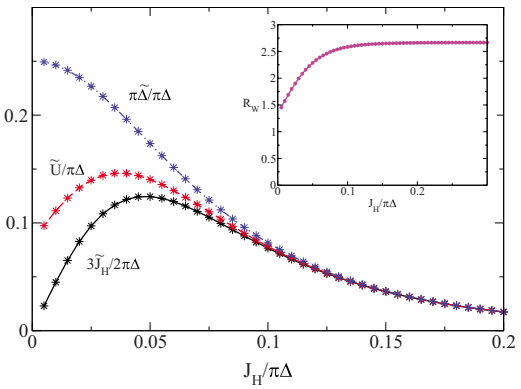

FIG. 8. (Color online) A plot of $\pi\tilde{\Delta}/\pi\Delta$, $\tilde{U}/\pi\Delta$ $3\tilde{J}_H/2\pi\Delta$ versus $J_H/\pi\Delta$ for $U/\pi\Delta=4.0$ and $\Delta=0.01$. There is a single renormalized energy scale when $J_H/\pi\Delta > 0.1$. The inset shows the corresponding Wilson ratio, $R_W=1+(\tilde{U}+\tilde{J}_H)/\pi\tilde{\Delta}$.

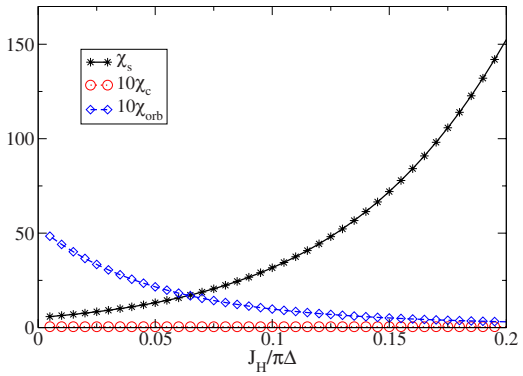

FIG. 9. (Color online) A plot of the spin susceptibility χ_s (units of $4\mu_B^2$), $10\times\chi_c$, where χ_c is the charge susceptibility, and the $10\times\chi_{orb}$, where χ_{orb} is the orbital susceptibility (units of $\mu_B^2/4$), versus $J_H/\pi\Delta$ for the same parameter set as in Fig. 8.

fact that the charge susceptibility is almost zero, due to the large value of U, $U/\pi\Delta=4.0$, means that the renormalized parameters must satisfy Eq. (28). This provides some insight into why the value of $\tilde{U}$ increases initially as J_H is switched on. For small J_H, the change in $\tilde{J}_H$ is almost linear whereas the change in $\pi\tilde{\Delta}$ is relatively small. Therefore to satisfy Eq. (28), $\tilde{U}$ must also increase almost linearly in this region. We can also see from Fig. 9 that the orbital susceptibility is small (multiplied by a factor 10 in the figure), and decreases monotonically as J_H increases.

In Fig. 10, we explore a different parameter regime. Here the parameters $\tilde{\Delta}$, $\tilde{U}$, and $3\tilde{J}_H/2$ are plotted for a range of values of U for $J_H/\pi\Delta=0.05$. We see that for this smaller value of J_H a large value of $U/\pi\Delta \sim 5.5$ is required before the orbital fluctuations are suppressed and the Kondo regime is achieved. We suggest that the explanation for this behavior is that a large U strongly renormalizes $\tilde{\Delta}$ so that the relatively weaker J_H is then sufficient to suppress the orbital fluctuations. In the large U limit, $\tilde{\Delta} \sim T_K$, it implies that the relevant criterion for estimating the effects of a relatively weak J_H is the ratio, J_H/T_K. We can see this more explicitly by calculating the Wilson ratio R_W in the localized limit when the charge susceptiblity is negligible and $\eta_c=0$. From Eqs. (22) and (25) we find

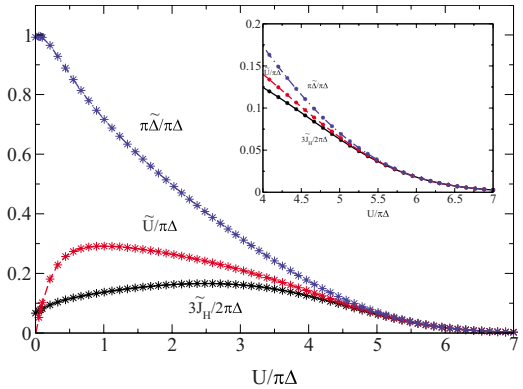

FIG. 10. (Color online) A plot of $\pi\tilde{\Delta}/\pi\Delta$, $\tilde{U}/\pi\Delta$, and $3\tilde{J}_H/2\pi\Delta$ versus $U/\pi\Delta$ for $J_H/\pi\Delta=0.05$ and $\Delta=0.01$.

$$R_W = 2\left[\frac{n\tilde{U} - (n-1)\tilde{J}_H}{(2n-1)\tilde{U} - 3(n-1)\tilde{J}_H}\right]. \quad (48)$$

So this ratio depends on $\tilde{J}_H/\tilde{U}$, and is valid for all values of J_H when $U/\pi\Delta$ is large. When J_H is very weak $\tilde{J}_H/\tilde{U} \sim J_H/T_K$, where T_K is the Kondo temperature for $J_H=0$. When $\tilde{J}_H$ is large $\tilde{J}_H/\tilde{U}=2/3$. An example of how the Wilson ratio changes with J_H, for large $U/\pi\Delta$, is shown in the inset of Fig. 8 for $n=2$ over the range $0<J_H/\pi\Delta\leq 0.2$ for $U/\pi\Delta=4$

It is of interest to compare the expression in Eq. (48) with the corresponding result of Nevidomskyy and Coleman[33] for the Wilson ratio of n single-channel Kondo models (coupling J) with the impurity spins coupled by a Hund's rule term (J_H), which takes the form,

$$R_W = 2\left[1 + \frac{(n-1)}{2(1+\eta)+1}\right], \quad (49)$$

where $\eta = U^*/J_H^* \sim J_H \gg T_K$, and U^*, J_H^* are renormalized channel-conserving and interchannel interactions associated with the Fermi-liquid fixed point, respectively, but which are not completely specified. With the assumption that $\eta \to 0$ in the limit of strong Hund's rule coupling this gives $R_W=2(n+2)/3$. If we rewrite the result in Eq. (48) in the form given in Eq. (49), we find an explicit expression for η in terms of $\tilde{U}$ and $\tilde{J}_H$,

$$\eta = \frac{n+1}{2}\left(\frac{2\tilde{U} - 3\tilde{J}_H}{2\tilde{J}_H - \tilde{U}}\right). \quad (50)$$

In this case when the Hund's rule coupling is strong, we get the result $\eta=0$ through cancellation as $2\tilde{U}=3\tilde{J}_H$. In the other limit $J_H=0$ ($\tilde{J}_H=0$), Eq. (50) gives $\eta=-(n+1)$. Substituting this value in Eq. (49) we recover the Wilson ratio for the Anderson model with $J_H=0$ in the large U regime as $R_W=2n/(2n-1)$ for the SU($2n$) model. When $J_H=0$ for the model used by Nevidomskyy and Coleman, $\eta \to \infty$, and $R_W=2$ corresponding to n independent SU(2) Kondo systems. This illustrates the fact that the two models are not equivalent, as we will discuss in more detail later.

Returning to the results for $J_H/\pi\Delta=0.05$ as a function of $U/\pi\Delta$ we see from the inset of Fig. 10 that, even though J_H is relatively small compared with $\pi\Delta$, when $U/\pi\Delta>5.5$ the value of T_K becomes sufficiently small such that $J_H \gg T_K$ and we enter a Kondo regime characterized by a single energy scale. In Fig. 11, we plot the Wilson χ_s/γ ratio, $R_W=1+(\tilde{U}+\tilde{J}_H)/\pi\tilde{\Delta}$, for the parameter set given in Fig. 10. It shows a steady increase from a value $R_W \sim 1$ for small U with a leveling off at $U/\pi\Delta \sim 5$ and then a convergence to the value $R_W=8/3$, corresponding to that of the localized $S=1$ two-channel Kondo model.

In the Kondo regime for the model with $J_H \neq 0$ with particle-hole symmetry we have $T_K=\pi\tilde{\Delta}/4$. This regime occurs when J_H is large enough so that the triplet state of the impurity has a much lower energy than the other two-particle impurity states. The effective coupling of this state to the conduction electrons, via virtual transitions to either single-particle or three-particle impurity states induced by the hybridization, leads to an exchange model of a localized spin 1 coupled to the two channels of conduction electrons with an effective antiferromagnetic exchange interaction $J_{eff}=4V^2/(U+3J_H)$. This in turn will lead to a J_H-dependent term in the Kondo temperature of the form $T_K \sim \exp(-a\pi^2 J_H/\pi\Delta)$, where a is a dimensionless numerical coefficient. This implies that in the Kondo regime T_K will vary exponentially with $J_H/\pi\Delta$. In Fig. 12, we plot T_K from the NRG results against $J_H/\pi\Delta$ and compare them with an exponential fit. The inset shows the plot of the logarithm of T_K, $\ln(T_K/\pi\Delta)$, versus $J_H/\pi\Delta$. It can be seen that the exponential form does fit well with the results for the Kondo range $J_H/\pi\Delta>0.1$ with the value $a=1.49$. There is a slight deviation for the largest values of J_H shown but the coefficient a depends on the range chosen for the curve fitting. There have been NRG calculations by Pruschke and Bulla[34] on an impurity model with a Hund's rule term, who find an exponential reduction in the width of the Kondo resonance in the impurity one-electron spectral density with increase in J_H, which corresponds at half filling to a exponential reduction in T_K.

For the n-channel Kondo model with Hund's rule coupling, Nevidomskyy and Coleman[33] have predicted a power

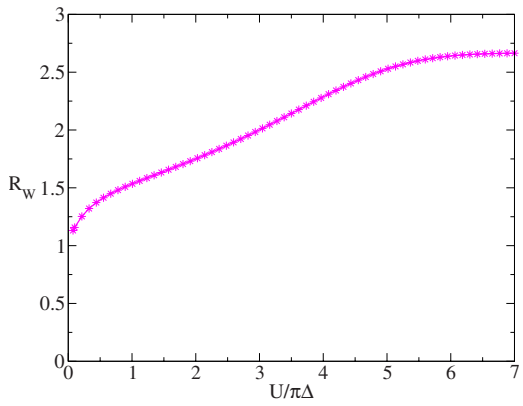

FIG. 11. (Color online) A plot of the Wilson ratio $R_W=1+(\tilde{U}+\tilde{J}_H)/\pi\tilde{\Delta}$ versus $U/\pi\Delta$ for $J_H/\pi\Delta=0.05$ and $\Delta=0.01$.

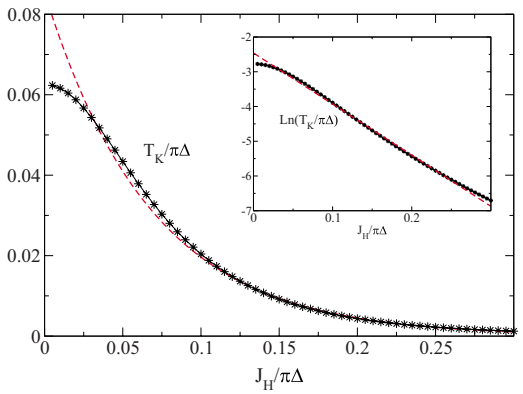

FIG. 12. (Color online) A plot $T_K/\pi\Delta$ (full curve) and $0.0854\exp(-1.49\pi^2 J_H/\pi\Delta)$ (dotted curve) versus $J_H/\pi\Delta$ for $U/\pi\Delta=4$ and $\Delta=0.01$. The inset shows the $\ln(T_K/\pi\Delta)$ and $-1.49\pi^2 J_H/\pi\Delta+\ln(0.0854)$.

law rather than an exponential dependence of T_K with J_H in the Kondo regime where the spins are completely coupled to give a total spin $S=n/2$, $T_K \sim J_H^{-(n-1)}$. We have a Kondo regime with a total spin $S=1$ for $U/\pi\Delta=4$ when $J_H/\pi\Delta > 0.1$, and the power-law behavior definitely does not agree with our numerical results, which show an exponential reduction with increase in J_H. However, there are differences between the models. When U is large, the Anderson model we use is not equivalent to the model of Nevidomskyy and Coleman. This can be seen clearly for $J_H=0$ electrons; when U is large our model becomes equivalent to a Coqblin-Schrieffer or SU($2n$) Kondo model with the operators in a $(2n)!/(n!)^2$ irreducible representation of the SU($2n$) group, while the model used by Nevidomskyy and Coleman becomes n independent SU(2) Kondo models. This is because the SU($2n$) Kondo model here includes orbital fluctuations. These are only suppressed by switching on the Hund's rule term, which also aligns the spins into a total spin $S=n/2$. In the Nevidomskyy and Coleman model the orbital fluctuations are not present, and the sole function of the Hund's rule term is to align the individual spins into a total spin $S=n/2$. This explains why in the case $J_H=0$, we obtain a Wilson ratio of $2n/(2n-1)$ in this case while the corresponding result for Nevidomskyy and Coleman model is 2, independent of n.

Nevidomskyy and Coleman consider the effect of the Hund's rule term in order to explain the trend observed in transition-metal impurity systems, that the Kondo temperature decreases sharply the larger the value of the impurity spin $S=n/2$. To make a comparison in our case between $S=1/2$ and $S=1$, on the assumption that the orbital fluctuations have been suppressed in each case, we need to compare the T_K for the $n=1$ model with that for the $n=2$ model. Due to the extra factor of 1/2 for $n=2$ in the exponential term in the expression given earlier for T_K for $J_H=0$, for the same value of U, $T_K[n=2] \gg T_K[n=1]$. When the reduction in $T_K[n=2]$ with J_H is included then there is a threshold value of J_H which must be achieved before the Kondo temperature of the $n=2$ model ($J_H \neq 0$) becomes less than that of the model with $n=1$. If we compare T_K for $n=1$ and $U/\pi\Delta=4$ with that for $n=2$ and $U/\pi\Delta=4$, we find that J_H/U must exceed a value ~ 0.05 for the T_K with $S=1$ to be smaller than that for $S=1/2$. This threshold value for $U/\pi\Delta=4$ corresponds to $J_H/T_K[S=1/2] \sim 30$. Once J_H exceeds this threshold value, the T_K for $S=1$ will decrease rapidly for larger values of J_H.

Using the renormalized parameters for values of $J_H/\pi\Delta=0.05$ and $J_H/\pi\Delta=0.15$ taken from Fig. 9 corresponding to $U/\pi\Delta=4$ and $\Delta=0.01$, we have evaluated the expressions for the dynamic spin susceptibility given in Eq. (39). The result for the real part is shown in Fig. 13. It illustrates the narrowing and height increase in the central peak with the larger value of J_H. In Fig. 14, the imaginary part of $\chi_s^{+-}(\omega)$ is shown. The marked increase in the change in the gradient through the origin for the larger value of J_H, can be explained as a consequence of the Korringa-Shiba relation given in Eq. (42).

IV. CONCLUSIONS

The point of this study here for the n-channel Anderson model has been to show how the renormalized perturbation

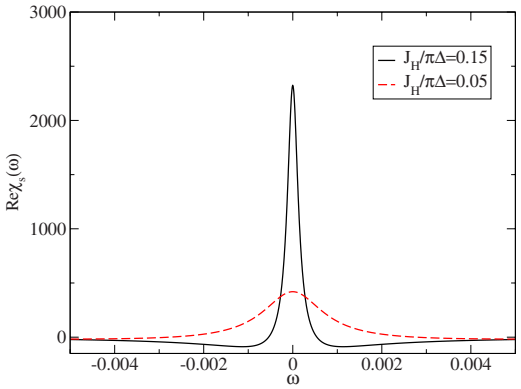

FIG. 13. (Color online) A plot of the real part of the dynamic spin susceptibility $\chi_s^{+-}(\omega)$ (in units of $8\mu_B^2$) for $J_H/\pi\Delta=0.05$ and $J_H/\pi\Delta=0.15$ with $U/\pi\Delta=4$ and $\Delta=0.01$.

approach (RPT) can provide an asymptotically exact way of calculating the low-temperature and low-frequency behavior of the model in all parameter regimes. There have been many previous studies of related multiorbital impurity models using a variety of approaches. The general n-channel Anderson model with finite U has not so far been solved using the Bethe ansatz, but there are exact solutions using this technique for the n-channel Kondo model coupled to a spin S (Refs. 29, 30, and 35) and the n-channel Anderson model in the infinite U limit. In the latter case the impurity occupation number is restricted to the range $n_d \leq 1$.[31] The main focus of the work on the n-channel Kondo model, however, has been on the overscreened case for $n \geq 2S$, where S is the spin of the impurity, as the model has a low-energy non-Fermi-liquid fixed point. Schlottmann and Sacramento,[36,37] however, have considered in detail the Bethe ansatz solution for the fully compensated case where $S=n/2$ and compared the results with the experimental data for the Kondo systems Fe in Cu and Ag, and Cr in Cu. There have been many NRG studies of multiorbital models, and this work has been surveyed in the NRG review article.[26] The concern in most of the NRG work has been with the calculation of the one-electron spectral densities, and mainly for the models without the Hund's rule term. There has been a DMFT-NRG study of a two-band Hubbard model by Pruschke and

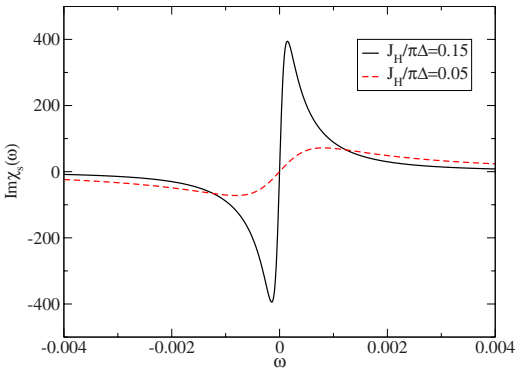

FIG. 14. (Color online) A plot of the imaginary part of the dynamic spin susceptibility $\chi_s^{+-}(\omega)$ (in units of $8\pi\mu_B^2$) for $J_H/\pi\Delta=0.05$ and $J_H/\pi\Delta=0.15$ with $U/\pi\Delta=4$ and $\Delta=0.01$.

Bulla,[34] which has a short section on the symmetric two-channel Anderson model. As in the results reported here, they found an an exponential reduction in the width of the Kondo resonance with J_H. There has also been a recent study for the $J_H=0$ model using the local moment approach, which includes NRG calculations for the case $n=2$,[22] and NRG studies of capacitively coupled quantum dots.[13]

The main feature of the RPT approach is that the calculations are carried out in terms of renormalized parameters which have a clear physical meaning in terms of the quasiparticles and their interactions. For the n-channel model, they correspond to renormalizations of the parameters, ϵ_d, Δ, U, and J_H, which specify the model. Asymptotically exact expressions can then be derived for the low-temperature behavior of the model in terms of these renormalized parameters. In the Kondo regime, all the renormalized parameters can be expressed in terms of a single renormalized energy scale, the Kondo temperature T_K. For the case $n=2$, we have been able to deduce the renormalized parameters from the low-lying excitations in an NRG calculation. The NRG results provide a comprehensive picture of the low-energy behavior of the model. As we have explicit expressions in Eqs. (20) and (22)–(24) for the specific-heat coefficient, spin, orbital, and charge susceptibilities at zero temperature, these quantities can be calculated simply by substituting the renormalized parameters into the relevant formulas. This procedure is very accurate and by passes the usual NRG method which involves a subtraction procedure to isolate the impurity component. In the Kondo regime, the results explicitly confirm the relations between the renormalized parameters predicted by the RPT.

Our numerical results have confirmed the importance of the effect of the Hund's rule coupling in reducing the Kondo temperature predicted by Nevidomskyy and Coleman,[33] who show experimental evidence for a correlation between a large decrease in Kondo temperature with the magnitude of the impurity spin for a number of Kondo systems. The Kondo resonance narrowing is more marked in our results, which show an exponential reduction, rather than the power-law dependence found by Nevidomskyy and Coleman. It should be noted, however, that the models are not equivalent, and, in particular, the Kondo coupling J of the individual spins in their model is independent of J_H whereas in starting from an Anderson model, we would have a J_H dependence in the effective value of J. We find that the Hund's rule coupling has to exceed a critical value for the Kondo temperature to decrease with an increase in the spin value from $S=1/2$ to $S=1$.

In setting up the RPT no approximation has been made, other than the assumption that the self-energy and its derivative are real and nondivergent at the Fermi level $\omega=0$. This means that there is the possibility of extending the results to higher temperatures and frequencies. Some preliminary results have been achieved by including diagrams beyond second order[11,38] for the single-channel model and this topic is currently being studied. The RPT in the Keldysh formalism can also be applied to nonequilibrium behavior and has been applied to the calculation of the nonlinear corrections to the differential conductance for a quantum dot,[39,40] including an arbitrary magnetic field.[41]

The RPT approach is not restricted to impurity models but the calculation of the renormalized parameters for lattice models presents more of a problem as the NRG method cannot in general be applied. However, for infinite dimensional lattice models one can use the DMFT to map the model into an effective impurity one so the NRG method can then be used. This approach has been used to calculate renormalized parameters for the one-band Hubbard and Hubbard-Holstein models.[42,43] The work presented here opens up the possibility of extending this method to the two-band Hubbard model with a Hund's rule coupling. We have found that the Hund's rule term plays an important role in enhancing the magnetic response in the twofold degenerate model. It is known that the single-band Hubbard model does not provide a basis for explaining the occurrence of ferromagnetism in $3d$ metals, as it predicts a ferromagnetic ground state only in a very restricted parameter regime, very close to half filling and for a value of U much greater than the band width. It is likely that the inclusion of the Hund's rule coupling is essential to describe ferromagnetism in $3d$ materials.

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APPENDIX

For the particle-hole symmetric model with $n=2$, the model given in Eq. (46) can be derived by taking account to order $|V|^2$ the effects of virtual excitations from the two-electron to the local one-electron and three-electron impurity states. We denote the one-electron basis states, $|1\uparrow\rangle$, $|1\downarrow\rangle$, $|2\uparrow\rangle$, and $|2\downarrow\rangle$, by $|\nu\rangle$ with $\nu=1,2,3,4$, respectively. The two-electron states we denote by $|\nu,\nu'\rangle$, with $\nu\neq\nu'$ and $|\nu',\nu\rangle$ represents the same state. This gives a six-dimensional basis set. In terms of the Hubbard operators $X_{(\nu,\nu'):(\nu'',\nu''')}=|\nu,\nu'\rangle\langle\nu'',\nu'''|$, the $Y_{\nu,\nu'}$ are given by

$$Y_{\nu,\nu'}=\sum_{\nu''\neq\nu,\nu''\neq\nu'}(-1)^{\alpha}X_{(\nu,\nu''):(\nu',\nu'')}, \tag{A1}$$

for $\nu'\geq\nu$, where $\alpha=1$ if $\nu<\nu''<\nu'$, otherwise $\alpha=0$. The $Y_{\nu',\nu}$ for $\nu'>\nu$ can be deduced from Eq. (A1) using $Y_{\nu',\nu}=(Y_{\nu,\nu'})^{\dagger}$.

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