Renormalized parameters and perturbation theory for an n-channel Anderson model
with Hund’s rule coupling: Asymmetric Case

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We explore the predictions of the renormalized perturbation theory for the n-channel Anderson model, both with and without Hund’s rule coupling, in the regime away from particle-hole symmetry. For the model with $n = 2$ we deduce the renormalized parameters from numerical renormalization group calculations, and plot them as a function of the local occupation of the impurity site $n_d$. From these we deduce the orbital, spin and charge susceptibilities, Wilson ratios and quasiparticle density of states at $T = 0$ in the different parameter regimes, which gives a comprehensive overview of the low energy behavior of the model. We compare the difference in Kondo behaviors at the points where $n_d = 1$ and $n_d = 2$. One unexpected feature of the results is the suppression of the charge susceptibility in strong correlation regime over the occupation number range $1 \leq n_d \leq 3$.

I. INTRODUCTION

In an earlier paper we applied a renormalized perturbation approach to study the low temperature behavior of an n-channel impurity Anderson model with a Hund’s rule exchange term. This form of perturbation theory is expressed in terms of renormalized parameters of the model which have to be determined. We calculated these parameters explicitly for the particle-hole symmetric model with $n = 2$ from numerical renormalization group (NRG) calculations. Here we extend that work to calculate the renormalizations of the parameters away from particle-hole symmetry. This enables us to compare the behavior of the model in regimes corresponding to different values of occupation number at the impurity site, $n_d$. These calculations reveal some unexpected features in the variation of the renormalizations with $n_d$. For example, when the Hund’s rule coupling $J_H = 0$ we find that the points of maximum renormalization do not coincide with integral values of $n_d$ except at half-filling. We also find a strong suppression of the charge fluctuations when the on-site interaction is strong in regimes which would be classified as intermediate or mixed valent. On substituting these renormalized parameters into formulæ derived from the renormalized perturbation theory (RPT), we can deduce the spin, orbital and charge susceptibilities, specific heat coefficient and Wilson ratios at $T = 0$ over the full range of the occupation number $n_d$. This gives a comprehensive picture of the low energy behavior of the model, both with and without the Hund’s rule exchange term.

We begin with a brief description of the model, and some of the results from the earlier work, which will be used here. References to this earlier paper will from here onwards be denoted by I. The Hamiltonian takes the form,

$$
\mathcal{H} = \sum_{m \sigma} \epsilon_{d m \sigma} d_{m \sigma}^{\dagger} d_{m \sigma} + \sum_{k m \sigma} \epsilon_{k m \sigma} c_{k m \sigma}^{\dagger} c_{k m \sigma} + \sum_{k m \sigma} (V_k d_{m \sigma}^{\dagger} c_{k m \sigma} + V_k^{\dagger} c_{k m \sigma}^{\dagger} d_{m \sigma}) + \mathcal{H}_d
$$

where $d_{m \sigma}^{\dagger}$, $d_{m \sigma}$, are creation and annihilation operators for an electron in an impurity state with total angular momentum quantum number $l$, and $z$-component $m = -l, -l + 1, \ldots, l$, where $2l + 1 = n$, the number of channels, and spin component $\sigma = \uparrow, \downarrow$. The creation and annihilation operators $c_{k m \sigma}^{\dagger}$, $c_{k m \sigma}$ are for partial wave conduction electrons with energy $\epsilon_{k m \sigma}$. The hybridization width is determined by the factor $\Delta m \sigma (\epsilon) = \pi \sum_k |V_k|^2 \delta (\epsilon - \epsilon_{k m \sigma})$, which we can take to be a constant $\Delta$ 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,

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

As well as the direct Coulomb interaction $U$ between the electrons, a Hund’s rule exchange term $J_H$ is included 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.

For the two-channel case $\mathcal{H}_d$ can be expressed in the form,

$$
\mathcal{H}_d = U \sum_{\sigma = 1, 2} n_{d \sigma} n_{d \sigma'} + U_{12} \sum_{\sigma, \sigma'} n_{d, 1 \sigma} n_{d, 2 \sigma'} - 2 J_H \mathbf{S}_{d, 1} \cdot \mathbf{S}_{d, 2},
$$

with a ferromagnetic Heisenberg exchange coupling $2J_H$ between the electrons in the different channels, and $U_{12} = U - 3J_H/2$.

The renormalized perturbation theory is formulated in terms of the renormalized values of the parameters, $\epsilon_d$, $\Delta$, $U$, and $J_H$, which specify the model. We denote these by $\tilde{\epsilon}_d$, $\Delta$, $\tilde{U}$, and $\tilde{J}_H$. They are defined in terms of the self-energy of the impurity Green’s function and the 4-vertices at zero frequency. We will not repeat the definitions here but refer to I. The impurity specific heat coefficient $\gamma$, the spin $\chi_s$, orbital $\chi_{orb}$, and charge $\chi_c$
susceptibilities at $T = 0$ (zero magnetic field) can all be expressed explicitly in terms of these parameters. The specific heat coefficient $\gamma$ is given by

$$\gamma = 2n\pi^2 \hat{\rho}^{(0)}(0)/3,$$

(4)

where $\hat{\rho}^{(0)}(\omega)$ is the free quasiparticle density of states per single spin and channel,

$$\hat{\rho}_{ms}^{(0)}(\omega) = \frac{\hat{\Delta}/\pi} { (\omega - \epsilon_d)^2 + \Delta^2 }.$$

(5)

The results for the spin susceptibility is given by

$$\chi_s = 2n\mu_B^2 \eta_s \hat{\rho}^{(0)}(0),$$

(6)

where

$$\eta_s = 1 + (\tilde{U} + (n - 1)\tilde{J}_H) \hat{\rho}^{(0)}(0).$$

(7)

Similarly for the orbital susceptibility,

$$\chi_{\text{orb}} = \frac{(n^2 - 1)\mu_B^2 \eta_{\text{orb}} \hat{\rho}^{(0)}(0)}{12},$$

(8)

where

$$\eta_{\text{orb}} = 1 + (\tilde{U} - 3\tilde{J}_H) \hat{\rho}^{(0)}(0),$$

(9)

and the charge susceptibility,

$$\chi_c = 2n\eta_c \hat{\rho}^{(0)}(0),$$

(10)

where

$$\eta_c = 1 - ((2n - 1)\tilde{U} - 3(n - 1)\tilde{J}_H) \hat{\rho}^{(0)}(0).$$

(11)

The total occupation of the impurity site $n_d$ at $T = 0$ is given by

$$n_d = 2 - \frac{4}{\pi} \tan^{-1} \left( \frac{\tilde{\epsilon}_d}{\Delta} \right),$$

(12)

which corresponds to the Friedel sum rule. Using the result in equation (12), we can derive an expression for $\hat{\rho}^{(0)}(0)$ in terms of the total occupation of the impurity site, $n_d$,

$$\hat{\rho}^{(0)}(0) = \frac{\sin^2(\pi n_d/2n)}{\pi \Delta}.$$

(13)

These results can all be shown to be exact for the model with the renormalized parameters as defined in I.

II. NRG Calculation of Parameters for $N=2$

To evaluate the formulae for the low temperature properties of the model we need the values for the renormalized parameters. As shown in I an accurate way of calculating these in terms of the bare parameters $\tilde{\epsilon}_d$, $\Delta$, $U$ and $J_H$, is from an analysis of the approach to the low energy fixed point of the Wilson numerical renormalization group calculation. This method can be applied for channel numbers $n = 1, 2$, but becomes progressively more difficult to impossible for larger values of $n$, due to the increase in the size of the matrices to be diagonalized. If the renormalized parameters are defined as a function of $N$, the number of NRG iteration steps, then the renormalized values correspond to the fixed point values for large $N$. We use this approach for the $n = 2$ model, as we did for the particle-hole symmetric case. In that case we could take $\tilde{\epsilon}_d = 0$, but here, in moving away from particle-hole symmetry, we need to determine the additional parameter $\epsilon_d$. In Fig. 1 we show a typical plot for the case $U/\pi \Delta = 4$, $J_H/\pi \Delta = 0.15$, $\pi \Delta = 0.01$ and $\epsilon_d/\pi \Delta = -3.574$. The renormalized parameters can be deduced accurately from the plateau regions that develop for large $N$. For more details we refer to I and the references therein.

A. SU(2n) Model $J_H = 0$

We first of all look at the results for the model with $J_H = 0$, which has SU(2n) symmetry. Our main interest will be in the strong correlation regime, where $U$ is large and the impurity electrons are almost localized, such that the charge susceptibility is suppressed. If we take $\eta_c = 0$ in Eq. (11) we find

$$\tilde{U} \hat{\rho}^{(0)}(0) = \frac{1}{(2n - 1)}.$$  

(14)

This implies that the effect of the quasiparticle interactions gets weaker the larger the channel index $n$, and goes to zero in the limit $n \rightarrow \infty$. Substituting the expression
we plot $4$ as a function of $U/\pi$ value for very accurate verification of the relation from Eq. (15) we get the result there is localization and a single energy scale for $\tilde{\Delta} = 1$ already shown from the NRG calculations for $n$ the points of integral valence $1)$. Wilson ratio, $R_W = \pi^2 \chi_s / 3 \mu_B^2 \gamma$, we find $R_W = 2n / (2n - 1)$ when we are in a localized regime.

For $n = 2$ we expect these relations to be satisfied at the points of integral valence $n_d = 1, 2, 3$. In I we have already shown from the NRG calculations for $n = 2$ that at the particle-hole symmetric point $n_d = 2$, the relation $U / \pi \Delta = 1/3$ in agreement with Eq. (15). For $n_d = 1, 3, \ldots$ from Eq. (15) we get the result $U / \pi \Delta = 2/3$. In Fig. 2 we plot $2\Delta / 3\Delta$, $U / \pi \Delta$, and the ratio $U / \pi \Delta$ for $n_d = 1$ as a function of $U / \pi \Delta$ for $\pi \Delta = 0.01$. It can be seen that there is localization and a single energy scale for $U / \pi \Delta > 4.5$, and the ratio $U / \pi \Delta$ asymptotically approaches the value $2/3$. For $U / \pi \Delta = 14$ we find $U / \pi \Delta = 0.66665$, a very accurate verification of the relation from Eq. (15) for $n_d = 1$ and $n = 2$.

![Fig. 2](image2.png)

**FIG. 2:** (Color online) A plot of $\tilde{U} / \pi \Delta$, $U / \pi \Delta$, $2\tilde{\Delta} / 3\Delta$ and $\tilde{U} / \pi \Delta$ the case $n_d = 1$ with $U / \pi \Delta$, $J_H = 0$ and $\pi \Delta = 0.01$

To look at the behavior more generally in the strong correlation regime, we have calculated the renormalized parameters for $U / \pi \Delta = 5$, $\Delta = 0.01$ over the full range of the occupation number $n_d$. The results for $\tilde{\epsilon}_d / \pi \Delta$, $\Delta / \Delta$ and $\tilde{U} / \pi \Delta$ are shown in Fig. 3. There are three distinct local minima in $\Delta$ at $n_d = 2$ and for values of $n_d$ slightly greater than 1 and slightly less than 3. This was to be expected, as the regions near integral values of $n_d$ for large $U$ correspond to localized Kondo regimes, and the dips in the values of $\Delta$ indicate a narrowing of the quasiparticle density of states at these points. It is an unexpected result, however, that minima away from the particle-hole symmetric point $n_d = 2$ are not precisely at $n_d = 1$ and $n_d = 3$. Also we find in the mixed valence regimes, $1 < n_d < 2$ and $2 < n_d < 3$, there is still some significant renormalization of $\Delta$. For $n_d < 0.7$ and $n_d > 3.3$, the values of $\tilde{\Delta}$ rapidly approach the bare value $\Delta$.

![Fig. 3](image3.png)

**FIG. 3:** (Color online) The renormalized parameters $\tilde{\epsilon}_d$, $\pi \tilde{\Delta}$, $\tilde{U}$ (in units of $\pi \Delta$ with $\Delta = 0.01$) as a function of the impurity occupation $n_d$ for $U / \pi \Delta = 5$ and $J_H = 0$.

In Fig. 4 we give the corresponding results for $\chi_s$ and $\chi_c$. The enhanced peaks in $\chi_s$ in the Kondo regimes near integral values of $n_d$ are as expected. It can be seen from Fig. 3 that the values of $\Delta$ at $n_d = 1, 2, 3$ are almost the same. The higher value of $\chi_s$ at $n_d = 2$, therefore, is due to the fact that at this point $\tilde{\epsilon}_d = 0$ giving a higher quasiparticle density of states compared with the peaks near $n_d = 1$ and $n_d = 3$. Again we note that the peaks in $\chi_s$ near $n_d = 1$ and $n_d = 3$ are not precisely at these integer values.

![Fig. 4](image4.png)

**FIG. 4:** (Color online) The spin susceptibility $\chi_s$ (units of $4\mu_B^2$) and the charge susceptibility $\chi_c$ as a function of the impurity occupation $n_d$ for $U / \pi \Delta = 5$ and $J_H = 0$.

The values of $\chi_c$ can be seen to be very small at $n_d = 2$ and near $n_d = 1, 3$. It is, however, rather small over the
the charge susceptibility not just for
This indicates that quasiparticle interaction suppresses
values of \( \eta \) in the mixed valence regimes
but the values are still very small. The Wilson ratio
seen that \( \eta \) is very small implies that impurity d-electrons
is equal to \( 0 \) for this model when \( \Delta = 0 \).
We plot \( \eta \), Eq. (15) versus \( n_d \) for \( U/\pi \Delta = 5 \) and \( J_H = 0 \).
In Fig. 5 we plot \( \eta \) and compare with the form given
on the right-hand side of Eq. (16). It can be seen that the two curves are in good agreement over the range from \( n_d = 0.9 \) to \( n_d = 3.1 \).

It is also of interest to compare the two integral valence cases, \( n_d = 1 \) and \( n_d = 2 \). In the Kondo regime for large \( U \), the models with \( n_d = 1 \) and \( n_d = 2 \) can both be mapped onto Coqblin-Schrieffer models of the form,

\[
\mathcal{H}_{CS} = J_{\text{eff}} \sum_{\nu,\nu',k,k'} Y_{\nu,\nu'} c_{k,\nu}^\dagger c_{k,\nu'} + \sum_{\nu,k} \epsilon_k c_{k,\nu}^\dagger c_{k,\nu},
\]

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

\[
[Y_{\nu,\nu'}, Y_{\nu'',\nu'''}] = Y_{\nu,\nu'''} \delta_{\nu',\nu''} - Y_{\nu'',\nu'} \delta_{\nu,\nu''},
\]

with \( \sum_{\nu} Y_{\nu,\nu'} = nI \). Though we are dealing with the model for the same value of \( n \), in this case \( n = 2 \), the models for \( n_d = 1 \) and \( n_d = 2 \), differ in that the operators transform according to different irreducible representations of SU(4). The case with \( n_d = 1 \) is the one originally considered by Coqblin and Schrieffer\(^4\), where the representation of the operators \( Y_{\nu,\nu'} \) is the fundamental representation of the group, which for the SU(4) group has dimension 4. On the other hand for \( n_d = 2 \), as we noted in I, the \( Y_{\nu,\nu'} \) operators correspond to a 6 dimensional irreducible representation of the SU(4) group. This is similar to a Heisenberg model, which can describe physical situations depending on the dimensionality of the irreducible representation used for the spin operators, 2S + 1 for a spin \( S \). In the general \( n \) channel model with \( r \) localized electrons the dimensionality of the irreducible representation of the operators in the Coqblin-Schrieffer model will be \((2n)!/(2n-r)!r!\).

More generally when \( n_d \leq 1 \), and \( U/\pi \Delta \gg 1 \), the model with \( J_H = 0 \) can be related to the \( N \)-fold degenerate, \( U = \infty \), Anderson model which has been applied to rare earth impurities such as Ce and Yb with \( N = 2n \). In this application the index \( \nu \) corresponds the \( z \)-component of total angular momentum, orbital plus spin \( m_J \), with \( N = 2j + 1 \), and \( j \) is the total angular momentum quantum number. The equation for the total angular momentum susceptibility \( \chi_j \) for this model is given by

\[
\chi_j = \frac{(g\mu_B)^2 j(j+1)}{3} N \eta_j \bar{\rho}(0),
\]

where \( g \) is the \( g \)-factor for coupling to the magnetic field and

\[
\eta_j = 1 + \bar{\rho}(0),
\]

while the equation for the charge susceptibility is the same as in Eq. (10) with \( 2n = N \). The Wilson ratio for the \( N \)-fold degenerate model (\( U = \infty \)) is defined as \( R_W = \pi^2 \chi_j j(j+1)(g\mu_B)^2 \gamma \); giving \( R_W = \eta_j = N/(N-1) \), which is the same as that we have for the SU(2n) model for \( N = 2n \).
In the localized limit when $U/\pi \Delta$ is large we have only one energy scale which we take to be the Kondo temperature $T_K$. For the $N$-fold degenerate, infinite $U$, Anderson model $T_K$ is defined such that $\chi = (g\mu B)^2 j(j+1)/3T_K$. This is equivalent to

$$T_K = \frac{2n-1}{4n^2 \tilde{\rho}(0)}.$$  \hspace{1cm} (21)

which we will take as a general definition for $T_K$ for the SU($2n$) model in the discussion here. It differs from the definition used in I by the factor $(2n-1)/n^2$.

On using Eq. (13) for $\tilde{\rho}(0)$, we find

$$T_K = \frac{\pi \Delta (2n-1)}{4n^2 \sin^2(\pi n_d/2n)}.$$  \hspace{1cm} (22)

We would expect this formula to apply only at or near the points of integer occupation of the impurity site, $n_d = 1, 2, 3$. However, for large $U/\pi \Delta$ we found localization and a Wilson ratio $R_K \approx 4/3$ over the complete range $1 \leq n_d \leq 3$. This means that we can define a Kondo temperature as a function of $n_d$ over this range. A plot of $T_K$ based on Eq. (22) is given in Fig. 7 for $n = 2$ and $U/\pi \Delta = 5, 10$ ($\Delta = 0.01$). There are three dips corresponding to a local minima for $T_K$ at $n_d = 2$ and near $n_d = 1, 3$. For the larger value of $U$ the outer minima move slightly closer towards $n_d = 1$ and $n_d = 3$.

![Figure 7](image1.png)

**FIG. 7:** (Color online) A plot of the Kondo temperature $T_K$, as defined in Eq. (22), as a function of $n_d$. The formula given in (22) is valid over the interval $0.9 < n_d < 3.1$ where $\tilde{\epsilon}_c \approx 0$.

We noted earlier that in the Kondo limit $n_d = 1$ and $n_d = 2$ are described by different Coqblin-Schrieffer models. They also have different values for the Kondo temperature $T_K$. In Fig. 8 we plot the Kondo temperatures $T_K$ for $n_d = 1$ and $n_d = 2$ for the range $5 \leq U/\pi \Delta \leq 14$ for $\pi \Delta = 0.01$. In I we fitted the $T_K$ for $n_d = 2$ to the exponential form, $T_K/\pi \Delta = \text{const} \times u \exp(-\pi^2 u/16+0.25/u)$ where $u = U/\pi \Delta$. The ratio of $T_K$ for $n_d = 1$ to that for $n_d = 2$ is shown in the inset of Fig. 8 and is seen to increase monotonically with $U/\pi \Delta$.

![Figure 8](image2.png)

**FIG. 8:** (Color online) The Kondo temperatures $T_K$ for $n_d = 1$ and $n_d = 2$ as a function of $U/\pi \Delta$ for $J_0 = 0$ and $\pi \Delta = 0.01$. The inset shows the corresponding ratio of $T_K[n_d = 1]/T_K[n_d = 2]$.

In the Kondo regime for general $n$ we can deduce the parameters $\tilde{\epsilon}_d$ and $\tilde{U}$ in terms of $T_K$,

$$\tilde{\epsilon}_d = T_K \frac{2n^2 \sin(\pi n_d/n)}{\pi(2n-1)}.$$  \hspace{1cm} (23)

$$\tilde{U} = \left( \frac{2n}{2n-1} \right)^2 T_K.$$  \hspace{1cm} (24)

Using Eq. (23) and (22) we can derive an explicit expression the quasiparticle density of states $\tilde{\rho}(0)(\omega)$ in the Kondo regime,

$$\tilde{\rho}(0)(\omega) = \frac{(2n-1)/4n^2 T_K}{\Omega - \cos(\pi n_d/2n)} + \sin^2(\pi n_d/2n).$$  \hspace{1cm} (25)

where $\Omega = \omega \pi (2n-1)/4T_K n^2 \sin(\pi n_d/2n)$. In applying the results in Eqs. (22) to (25) to the infinite $U$ model we must take $n_d = 1$.

We can contrast the quasiparticle density of states in the case of half-filling, $n_d = n$, with that for $n_d = 1$. In the former case, $\tilde{\epsilon}_d = 0$ and the quasiparticle density of states is symmetrically placed about the Fermi level, and for large $n$, $\tilde{\rho}(0)(\omega)$ takes the approximate form,

$$\tilde{\rho}(0)(\omega) \approx \frac{2n T_K/\pi^2}{\omega^2 + (2n T_K/\pi)^2}.$$  \hspace{1cm} (26)

For $n_d = 1$ and $n > 1$, on the other hand, the quasiparticle peak is asymmetrically placed about the Fermi level. For large $n$, $\tilde{\rho}(0)(\omega)$ takes the approximate form,

$$\tilde{\rho}(0)(\omega) \approx \frac{T_K/2n}{(\omega - T_K)^2 + (\pi T_K/2n)^2}.$$  \hspace{1cm} (27)
and in the limit \( n \to \infty \) collapses to a delta-function at a point \( T_K \) above the Fermi level. This asymmetry with respect to the Fermi level for \( n_d = 1, n > 1 \), is required by the Friedel sum rule, because if \( n_d = 1 \), the quasiparticle density of states must be such that has only a fraction \( 1/2n \) is filled when integrated up to the Fermi level.

![Graph](image)

**FIG. 9:** (Color online) A comparison of the quasiparticle density of states \( \rho^{(0)}(\omega) \) for \( n_d = 2 \) and \( n_d = 1 \) for \( U/\pi \Delta = 5 \), \( J_H = 0 \) and \( \Delta = 0.01 \)

In Fig. 9 we compare the quasiparticle density of states for \( n_d = 1 \) and 2 for \( U/\pi \Delta = 5 \). We see that the peak in the case \( n_d = 1 \) is shifted slightly above the Fermi level so that the Friedel sum rule is satisfied in terms of the quasiparticles. This shift has physical consequences. If we ignore the effects of the quasiparticle interactions, which becomes an increasingly good approximation as the channel index \( n \), we can estimate the low temperature and low magnetic field corrections to the spin susceptibility from a free quasiparticle calculation. The \( T^2 \) and \( H^2 \) correction to the spin susceptibility, as well as the \( T^3 \) correction of the impurity specific heat contribution from this calculation are proportional to

\[
\left( \frac{\rho^{(0)''}(0)}{\rho^{(0)'(0)}} \right) - \left( \frac{\rho^{(0)''}(0)}{\rho^{(0)'(0)}} \right) = \frac{2(\epsilon_d^2 - \Delta^2)}{2(\epsilon_d^2 + \Delta^2)^2}, \tag{28}
\]

where \( \rho^{(0)'}(0) \) and \( \rho^{(0)''}(0) \) are the first and second derivatives of \( \rho^{(0)}(\omega) \) evaluated at \( \omega = 0 \). If \( |\epsilon_d| < \Delta \), which is the case when \( \epsilon_d = 0 \), then this coefficient is negative. However, when the quasiparticle density of states becomes asymmetric about the Fermi level such that \( |\epsilon_d| > \Delta \) it changes sign to become positive. As the susceptibility must eventually decrease at high temperatures and in high magnetic fields, this implies that there must be a peak in \( \chi_s(T) \) and \( \chi_s(H) \). Such a peak in found in the exact Bethe ansatz solutions for the \( N \)-fold degenerate, infinite \( U \), Anderson model for \( N > 2^{5,6,8} \), and this simple argument provides a qualitative explanation for this behavior. The form of the quasiparticle density of states in the vicinity of the Fermi level also affects the thermopower. The thermopower due to the impurity is proportional to the gradient of the quasiparticle density of states at the Fermi level; it is zero when the quasiparticle density of states is symmetrical about the Fermi level but large when there is narrow peak just above the Fermi level.

It is also possible that shift in the peak in the quasiparticle density of states, which for \( n = 2 \) will be to above the Fermi level for \( n_d = 1 \) and below the Fermi level for \( n_d = 3 \), may explain why the local minima in renormalized parameters and the peaks in the spin susceptibility do not occur at precisely at \( n_d = 1 \) and \( n_d = 3 \), but in one case slightly greater than \( n_d = 1 \) and in the other slightly less than \( n_d = 3 \).

### B. Model with \( J_H \neq 0 \)

We now consider the case with Hund’s rule coupling away from particle-hole symmetry. In Fig. 10 we show the renormalized parameters \( \chi_{orb} \) and \( \eta_s \) in Fig. 11 that at and very close to \( n_d = 2 \) the orbital susceptibility is also suppressed, so equating \( \eta_{orb} \) to zero from Eq. (29) we find

\[
3(\tilde{U} - \tilde{J}_H)\rho^{(0)}(0) = 1. \tag{29}
\]

In the discussion of the SU(2n) model, where \( J_H = 0 \), this condition left only one independent renormalized parameter, which we could take as the Kondo temperature. However, when \( J_H \neq 0 \), we are left with two renormalized parameters, so we cannot in this case define a Kondo temperature from this equation alone. We see from Fig. 11 that at and very close to \( n_d = 2 \) the orbital susceptibility is also suppressed, so equating \( \eta_{orb} \) to zero from Eq. (29) we find

\[
(3\tilde{J}_H - \tilde{U})\rho^{(0)}(0) = 1. \tag{30}
\]

At this point we have a single energy scale and can define a Kondo temperature via \( \chi_s = (g\mu_B)^2S(S+1)/3T_K \) for a spin \( S = 1 \), which is such that

\[
\pi \Delta = \tilde{U} = \frac{3}{2} \tilde{J}_H = 4T_K. \tag{31}
\]
and ξ_d = 0 from particle-hole symmetry. At this point the Wilson ratio R_W = η_s = 8/3, as can seen in Fig. 11.

The particle-hole symmetric case with n_d = 2 is discussed more fully in I.

In Fig. 12 we show the renormalized parameters as a function of n_d for smaller values of U and J_H, U/πΔ = 2 and J_H/πΔ = 0.05. The values of ξ_d, Δ, U are similar to the case with J_H = 0 shown in Fig. 5. In this case, in contrast to the previous example, J_H has a maximum at n_d = 2 rather than a minimum. For this smaller value of U, the renormalized value U is rather flat in most of the range from n_d = 1 to n_d = 3. In Fig. 13 we show the corresponding values for η_s, η_orb, and η_c. It shows that, even for this smaller value of U, there is some suppression of the charge susceptibility by the quasiparticle interactions. There is also some enhancement of χ_s and a commensurate reduction in η_orb as the particle-hole symmetric point n_d = 2 is approached.

In Fig. 14 we show the renormalized parameters with the same value of J_H (J_H/πΔ = 0.05) and a larger value of U, U/πΔ = 4. It can be seen that the effect of increasing U is to induce a rather shallow minimum in J_H at n_d = 2, and also in U. In Fig. 15 we give the corresponding values for η_s, η_orb, and η_c. It can be seen that, despite using the same value of J_H, η_s is enhanced and η_orb is reduced in the central region for the larger value of U. This indicates that the enhancement of η_s does not scale in proportion to J_H/U, but that J_H is more effective in suppressing the orbital fluctuations when the charge fluctuations are suppressed by a larger value of U.

In Fig. 16 we compare the quasiparticle density of states at n_d = 1 and n_d = 2 for U/πΔ = 2, 4, J_H = 0.05 and πΔ = 0.01. It illustrates both the shift in the peak the Kondo resonance to above the Fermi level for n_d = 1, the enhancement of the density of states at the Fermi level, and the narrowing of the resonance for the larger value of U.

Finally in Fig. 17 we compare the spin susceptibilities as a function of n_c calculated for the three sets of renormalized parameters given in Figs. 10, 12, and 14. The spin susceptibility is considerably enhanced near particle-hole symmetry for the case J_H/πΔ = 0.15 compared with that for J_H/πΔ = 0.05 and the same value of U (U/πΔ = 4). It also illustrates the more modest enhancement of χ_s for the larger value U/πΔ = 4 compared with the case for U/πΔ = 2 and the same value of J_H (J_H/πΔ = 0.05).

III. CONCLUSIONS

The combination of the renormalized perturbation theory with explicit calculations of the renormalized parameters from the numerical renormalization group for n = 2 have given us a comprehensive picture of the low energy behavior of the n-channel Anderson model, with and without a Hund’s rule coupling term. One or two features of these results deserve some additional discussion.

One surprising feature revealed by the NRG calculations of the renormalized parameters is the suppression of the impurity charge fluctuations over the whole range 1 ≤ n_d ≤ 3 for large U. At the points n_d = 1, 2, 3 for large U, in the atomic limit the impurity levels are well away from the Fermi level, and the quasiparticle resonance at the Fermi level is a many-body effect induced by the spin fluctuations. In intermediate valent situation between n_d = 1 and n_d = 2, and similarly between n_d = 2 and n_d = 3, in the atomic limit there are atomic excitation levels at the Fermi level, so once the hybridization is included one might expect the electrons
to jump on and off the impurity site relatively freely giving a largely unrenormalized charge susceptibility. The fact that $\eta_c$ is very small in this range suggests that there is a binding energy of electrons at the impurity site which suppresses the local charge fluctuations, even in these intermediate valent regimes. Presumably at temperatures much greater than this binding energy, the mobility of the electrons in these intermediate valence regimes will be restored. This topic deserves further investigation.

Another feature of the model that deserves some comment is the behavior in the large $n$ limit. We can contrast the situations for the SU(2n) model when we are in the Kondo regime at half-filling when $n_d = n$, with that for the model when $n_d = 1$. This latter situation corresponds to the infinite $U$ Anderson model used to describe rare earth impurities. It can be seen from Eq. (14) that in the $n_d$ limit.

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FIG. 12: (Color online) The renormalized parameters $\tilde{\epsilon}_d$, $\tilde{\Delta}$, $\tilde{U}$ and $\tilde{J}_H$ (in units of $\pi \Delta = 0.01$) as a function of the impurity occupation $n_d$ for $U/\pi \Delta = 2$ and $J_H/\pi \Delta = 0.05$.

FIG. 13: (Color online) The coefficients $\eta_s (= R_W$, Wilson ratio), $\eta_{orb}$, and $\eta_c$ as a function of the impurity occupation $n_d$ for $U/\pi \Delta = 2$ and $J_H/\pi \Delta = 0.05$.

FIG. 14: (Color online) The renormalized parameters $\tilde{\epsilon}_d$, $\tilde{\Delta}$, $\tilde{U}$ and $\tilde{J}_H$ (in units of $\pi \Delta = 0.01$) as a function of the impurity occupation $n_d$ for $U/\pi \Delta = 4$ and $J_H/\pi \Delta = 0.05$.

FIG. 15: (Color online) The coefficients $\eta_s (= R_W$, Wilson ratio), $\eta_{orb}$, and $\eta_c$ as a function of the impurity occupation $n_d$ for $U/\pi \Delta = 4$ and $J_H/\pi \Delta = 0.05$.

FIG. 16: (Color online) The quasiparticle density of states $\tilde{\rho}^{(0)}(\omega)$ for $J_H/\pi \Delta = 0.05$, $U/\pi \Delta = 2, 4$ and $n_d = 1, 2$. 
limit \( n \to \infty \), the effects of the interactions between the quasiparticles go to zero as \( \bar{U} \tilde{\rho}(0) \to 0 \). The quasiparticle interaction \( \bar{U} \) given by Eq. (24) remains finite in this limit. The product \( \bar{U} \tilde{\rho}(0) \) tends to zero in this case, where \( n_d = 1 \), because \( \tilde{\rho}(0) \to 0 \). This contrasts with the situation at half-filling where, as \( n \to \infty \), the spin susceptibility \( \chi_s \) must scale with \( n \), so in taking the limit \( n \to \infty \), \( nT_k \) must be kept constant. Hence, in this limit \( \tilde{\rho}(0) \) remains finite and \( \bar{U} \to 0 \). These different scenarios reflect that the filling of the quasiparticle density of states must satisfy the Friedel sum rule so that when \( n_d = n \) it must span the Fermi level symmetrically, while when \( n_d = 1 \), the Fermi level must lie in the tail of the quasiparticle density of states to give a filling factor in each spin and channel of \( 1/2n \). These differences have physical consequences for the low temperature and magnetic field dependence of the susceptibility, giving a low energy peak when the Fermi level lies in the tail of the quasiparticle density of states, and also an enhanced thermopower.

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