1/\(N - 1\) expansion for a finite \(U\) Anderson model away from half-filling

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We apply recently developed 1/\(N - 1\) expansion to a particle-hole asymmetric SU(\(N\)) Anderson model with finite Coulomb interaction \(U\). To leading order in 1/\(N - 1\) it describes the Hartree-Fock random phase approximation (HF-RPA), and the higher-order corrections describe systematically the fluctuations beyond the HF-RPA. We show that the next-leading order results of the renormalized parameters for the local Fermi-liquid state agree closely with the numerical renormalization group results at \(N = 4\). It ensures the reliability of the next-leading order results for \(N \geq 4\), and we examine the \(N\) dependence of the local Fermi-liquid parameters. Our expansion scheme uses the standard Feynman diagrams, and has wide potential applications.

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I. INTRODUCTION

Exploring the ground state and the low-energy excitations of strongly correlated electron systems is one of the fundamental subjects of quantum many-body theory. The low-lying energy states determine not only equilibrium properties but nonequilibrium transport deviating from the linear response. For instance, in quantum dots the universal Kondo behavior of the steady current in terms of the quasi-particles of a local Fermi liquid.

The universal behavior has been studied in more general situations with the orbital degeneracy. The essential feature of the universality in this case may be deduced from the low-energy states of the \(N\)-fold degenerate Anderson impurity. The exact numerical renormalization group (NRG) approach was successfully applied to this model for small degeneracies \(N \leq 4\) which for \(N = 2\) corresponds to the spin degeneracy. However, alternative approaches are required for large degeneracies \(N \geq 4\).

The conventional 1/\(N\) expansion, or non-crossing approximation (NCA), is one of such approaches. This and related approximations are based on the perturbation theory with respect to the hybridization matrix element \(V\) between the impurity and conduction band. They treat mainly the electron filling less than one electron in \(N\) orbitals, assuming an infinite Coulomb interaction \(U\). Extensions of the methods of this category to the case of finite \(U\) have been developed, also on the basis of the perturbation theory in \(V\), using the slave-boson or the resolvent technique. However, in order to explore a wide range of the electron fillings and of the other parameters, it is still necessary to develop different approaches applicable to the low-energy excitations.

In a previous paper, we proposed a completely different approach, using a scaling that takes \(u = (N - 1)/U\) as an independent variable instead of the Coulomb interaction \(U\) alone. The factor \(N - 1\) appears naturally as it represents the number of interacting orbitals, excluding the one prohibited by the Pauli principle. With this scaling the perturbation series in \(U\) can be reorganized as an expansion in powers of 1/\(N - 1\). This can be carried out by using a standard Feynman diagrammatic technique for the fermions with two-body interactions. Specifically, diagrammatic classification, similar to the one for the \(N\)-component \(\varphi^4\) model for critical phenomena, is applicable with an extension that takes into account the fermionic anticommutation relation. We calculated the renormalization parameters for the quasi-particles up to order 1/\(N - 1\)^2 at half-filling, and confirmed that the results agree closely with the NRG results for \(N = 4\). It enabled us to clarify the \(N\) dependence of the nonequilibrium Kondo behavior for \(N > 4\).

In this paper, we apply this approach to away from half-filling, and examine the ground-state properties. To this end, we choose the unperturbed Green’s function such that it includes the level shift due to the \(\omega = 0\) component of the self-energy, which at zeroth order is given by the Hartree-Fock (HF) approximation. The first order contributions in the 1/\(N - 1\) expansion consists of the vertex and self-energy corrections, which are equivalent to those of the random phase approximation (RPA). The higher order contributions systematically capture the correlation effects beyond the HF-RPA. We show that the order 1/\(N - 1\)^2 results of the renormalized parameters agree well to those of the NRG also in the particle-hole asymmetric case. It ensures an early convergence of the 1/\(N - 1\) expansion for \(N \geq 4\). With this approach, we also examine the \(N\) dependence of the local Fermi-liquid parameters. Our expansion procedure, using the standard Feynman diagrams, is quite general. It can be applied to the Keldysh formalism, and to lattice systems such as the Hubbard model.

This paper is organized as follows. We describe the model and the basic idea of the scaling of the Coulomb interaction \(U\) in Sec. \[\text{III}\]. The diagrammatic classification for the leading and next-leading order terms in 1/\(N - 1\) expansion is explained in Sec. \[\text{III}\]. The numerical results for the renormalized parameters are presented in Sec. \[\text{IV}\]. A brief summary is given in Sec. \[\text{V}\].
II. MODEL AND FORMULATION

We consider the SU\((N)\) impurity Anderson model with finite interaction \(U\), given by
\[ \mathcal{H} = \mathcal{H}_d + \mathcal{H}_c + \mathcal{H}_V + \mathcal{H}_U, \]
where
\[ \mathcal{H}_d = \sum_{m=1}^N E_d \eta_{dm}, \quad \mathcal{H}_c = \sum_{m=1}^N \int_{-D}^D d\epsilon \, c^\dagger_{m\epsilon} c_{m\epsilon}, \]
\[ \mathcal{H}_V = \sum_{m \neq m'} U \left[ \langle n_{dm} - \langle n_{dm} \rangle \rangle \langle n_{d'm'} - \langle n_{d'm'} \rangle \rangle \right], \]
\[ \mathcal{H}_V = \sum_{m=1}^N V(d^\dagger m \psi_m + \text{H.c.}) , \quad \psi_m = \int_{-D}^D d\epsilon \sqrt{\rho} c_{m\epsilon}, \]
\[ E_d = \epsilon_d + \langle n_{dm} \rangle \langle N - 1 \rangle U, \]
where \(d^\dagger m\) is the creation operator for an electron with energy \(\epsilon_d\) and orbital \(m\) \((= 1, 2, \ldots, N)\) in the impurity site, and \(n_{dm} = d^\dagger m d_m\). The operator \(c^\dagger_{m\epsilon}\) creates a conduction electron that is normalized as \(\langle c_{m\epsilon}, c^\dagger_{m\epsilon'} \rangle = \delta_{m\epsilon, m'\epsilon}\). The hybridization energy scale is given by \(\Delta = \pi \rho V^2\) with \(\rho = 1/(2D)\). We consider the parameter region where \(\max (\Delta, |\epsilon_d|, U) \ll D\).

We use the imaginary-frequency Green’s function that takes the form for \(|\omega| \ll D\),
\[ G(i\omega) = \frac{1}{i\omega - E_d + i\Delta \text{sgn} \omega - \Sigma(i\omega)}, \]
where \(\Sigma(i\omega)\) is the self-energy due to \(\mathcal{H}_U\). The ground-state average of the local charge can be deduced from the phase shift \(\delta \equiv \cot^{-1}(E_d^*/\Delta)\) with \(E_d^* \equiv E_d + \Sigma(0)\), using the Friedel sum rule \(\langle n_{dm} \rangle = \delta / \pi\). The derivative of \(\Sigma(i\omega)\) determines the renormalized parameters \(\tilde{\gamma} \equiv 1 - \partial \Sigma(i\omega)/\partial (i\omega)|_{\omega=0}, \tilde{\epsilon}_d \equiv E_d^* / \tilde{\gamma}\), and \(\Delta \equiv \delta \Delta\). Furthermore, using the Ward identities, the enhancement factor for spin and charge susceptibilities, \(\tilde{\chi}_s \equiv \tilde{\chi}_{mm^\prime} - \tilde{\chi}_{mm}\) and \(\tilde{\chi}_c \equiv \tilde{\chi}_{mm^\prime} + (N - 1) \tilde{\chi}_{mm},\) can be expressed in terms of the renormalization \(\tilde{\gamma}\) and the vertex function \(\Gamma_{mm^\prime;m^\prime\prime} (i\omega_1, i\omega_2; i\omega_3, i\omega_4)\) for \(m \neq m'\),
\[ \tilde{\chi}_{mm^\prime} = \tilde{\gamma}, \quad \tilde{\chi}_{mm} = -\frac{\sin^2 \delta}{\pi \Delta} \Gamma_{mm^\prime;m^\prime\prime} (0, 0; 0, 0). \]

The residual interaction between the quasi-particles is also given by \(\tilde{U} \equiv 2 \Gamma_{mm^\prime;m^\prime\prime} (0, 0; 0, 0)\) for \(m \neq m'\).

We showed in the previous work that it is essential for \(N > 2\) to scale the Coulomb interaction by multiplying a factor \(N - 1\) in the particle-hole symmetric case. Away from half-filling, it is more natural to include an additional factor \(\sin^2 \delta\) such that
\[ K^* \equiv g \sin^2 \delta, \quad g \equiv \frac{(N - 1) U}{\pi \Delta}, \]
as the local density of states at the impurity site is given by \(-\frac{1}{\pi} \text{Im} G(i0^+) = \sin^2 \delta/\pi \Delta\). Similarly, we introduce the renormalized version of the scaled coupling constant,
\[ \tilde{K} \equiv \tilde{g} \sin^2 \delta, \quad \tilde{g} \equiv \frac{(N - 1) \tilde{U}}{\pi \Delta}. \]
The Wilson ratio \(R\) and that for the charge sector can be expressed in terms of the renormalized coupling \(\tilde{K}\),
\[ R \equiv \frac{\tilde{\gamma}}{\gamma} = 1 + \frac{\tilde{K}}{N - 1}, \quad \frac{\tilde{\gamma}}{\gamma} = 1 - \tilde{K}. \]
Conversely, it can also be written as \(\tilde{K} = (N - 1)(R - 1)\).

By definition, \(\tilde{K}\) is bounded in the range \(0 \leq \tilde{K} \leq 1\), and approaches \(\tilde{K} \rightarrow 1\) when the charge fluctuation is suppressed \(\tilde{\chi}_c \rightarrow 0\). At half-filling \(\epsilon_d = -(N - 1)U/2\) and \(E_d = 0\), it has been confirmed that \(\tilde{K}\) varies in a narrow region as \(N\) increases, and converges rapidly to the RPA value that is asymptotically exact in the \(N \rightarrow \infty\) limit.

Away from half-filling, the renormalized impurity level \(E_d^*\) determines the charge distribution near the impurity, and should be calculated in an optimal way. We treat this problem by taking the unperturbed Green’s function such that
\[ G_0(i\omega) = \frac{1}{i\omega - E_d^* + i\Delta \text{sgn} \omega}. \]

In this setup, the energy shift due to \(\Sigma(0)\) is included in the unperturbed part of the Hamiltonian, defined by
\[ \mathcal{H}_0 = \mathcal{H}_d + \mathcal{H}_c + \mathcal{H}_V + \sum_m \Sigma(0) n_{dm}, \]
and it is subtracted in the perturbation Hamiltonian
\[ \mathcal{H}_U = \mathcal{H}_U - \sum_m \lambda n_{dm}. \]

Here, the counter term is defined formally by \(\lambda = \Sigma(0)\). Then, the full Green’s function defined in Eq. (11) can be rewritten in the form
\[ G(i\omega) = \frac{1}{i\omega - E_d^* + i\Delta \text{sgn} \omega - \Sigma(i\omega)}. \]

The redefined self-energy \(\Sigma(i\omega)\) represents the corrections due to \(\mathcal{H}_U\), and can be calculated perturbatively as a function of \(E_d^*\) and \(\lambda\). These two parameters can be determined through the renormalization condition
\[ \Sigma(0) = 0, \]
and Eq. (11) that can be rewritten, using the Friedel sum rule, as
\[ \frac{\xi_d}{\Delta} = \frac{E_d^* - \lambda}{\Delta} + g \tan^{-1} \left( \frac{E_d^*}{\Delta} \right), \]
where \(\xi_d = \epsilon_d + (N - 1)U/2\). At half-filling \(\xi_d = 0\), both of the two parameters vanish, \(E_d^* = 0\) and \(\lambda = 0\).

III. 1/(N − 1) EXPANSION

The perturbation expansion with respect to \(\mathcal{H}_U\) can be classified according to the power of \(1/(N - 1)\), by
Thus at zero order, the counter term vanishes each order in the 1 of the renormalization condition Eq. (13) is satisfied to and the coefficient \( \lambda \) is determined by Eq. (14), which in this case gives

\[ \lambda = \sum_{k=0}^{\infty} \frac{\lambda_k}{(N-1)^k} , \]

and the coefficient \( \lambda_k \) is determined by the requirement of the renormalization condition Eq. (13) is satisfied to each order in the \( 1/(N-1) \) expansion.

A. Zeroth order

By construction, the tadpole diagrams and the contributions arising from the bilinear part of \( H_U \) defined in Eq. (2), i.e., \( -U \sum_{m \neq m'} \sum_{n,d,m} \langle n|d|m\rangle \cdot n_{dm} \), cancel each other. Thus at zero order, the counter term vanishes \( \lambda = 0 \), and \( E_d^* \) is determined by Eq. (14), which in this case gives the HF value,

\[ \frac{\xi_d}{\Delta} = \frac{E_d^*}{\Delta} + g \tan^{-1} \left( \frac{E_d^*}{\Delta} \right) . \]

Note that the corrections due to the RPA are still not included in the zeroth order.

B. Leading order

The leading order corrections in the \( 1/(N-1) \) expansion arise from a series of the bubble diagrams of the RPA type indicated in Fig. 1 and can be expressed in the form

\[ U_{\text{bub}}(i\omega) = \frac{\phi(i\omega)}{N-1} + \frac{g \pi \Delta \Pi(i\omega)}{(N-1)^2} + O \left( \frac{1}{(N-1)^3} \right) , \]

\[ \phi(i\omega) = \frac{g \pi \Delta}{1 + g \pi \Delta \chi_0(i\omega)} \] \( \Pi(i\omega) \equiv \chi_0(i\omega) \phi(i\omega) . \)

The precise form of \( U_{\text{bub}}(i\omega) \) and \( \chi_0(i\omega) \) are provided in Appendix A. The propagator \( U_{\text{bub}}(i\omega) \) contains also the higher order contributions in the \( 1/(N-1) \) expansion. This is because the orbital indices for adjacent bubbles have to be different due to the Pauli exclusion, and thus the summations over internal \( m \)’s for the fermion loops are not independent. The order \( 1/(N-1) \) terms of \( \Gamma_{mnm'}(0,0;0,0) \) arises from the first diagram in choosing the scaled interaction \( g \) as an independent variable instead of bare \( U \). The counter term can also be expanded such that

\[ \lambda = \sum_{k=0}^{\infty} \frac{\lambda_k}{(N-1)^k} , \]

and the coefficient \( \lambda_k \) is determined by the requirement of the renormalization condition Eq. (13) is satisfied to each order in the \( 1/(N-1) \) expansion.

By construction, the tadpole diagrams and the contributions arising from the bilinear part of \( H_U \) defined in Eq. (2), i.e., \( -U \sum_{m \neq m'} \sum_{n,d,m} \langle n|d|m\rangle \cdot n_{dm} \), cancel each other. Thus at zero order, the counter term vanishes \( \lambda = 0 \), and \( E_d^* \) is determined by Eq. (14), which in this case gives the HF value,

\[ \frac{\xi_d}{\Delta} = \frac{E_d^*}{\Delta} + g \tan^{-1} \left( \frac{E_d^*}{\Delta} \right) . \]

Note that the corrections due to the RPA are still not included in the zeroth order.

C. Next leading order

Fluctuations beyond the RPA enter through the next-leading and higher order terms in the \( 1/(N-1) \) expansion. In the particle-hole asymmetric case, the order \( 1/(N-1)^2 \) contributions to \( \Gamma_{mm'nmm'}(0,0;0,0) \) arise from the diagrams shown in Figs. 3 and 4 and also from the order \( 1/(N-1)^2 \) order component of \( U_{\text{bub}}(i\omega) \) shown in the first diagram of Fig. 2, i.e., the second term in

\[ \lambda = \Sigma(1/N')(i\omega) - \lambda + O \left( \frac{1}{N^2} \right) . \]

Note that \( \pi \Delta \chi_0(0) = 1/[1 + (E_d^*/\Delta)] \) also equals \( \sin^2 \delta \). Equation (19) determines the Wilson ratio \( R \), defined in Eq. (9), to order \( 1/(N-1) \).

The leading order self-energy due to \( \tilde{H}_U \) arises from the second and third diagrams in Fig. 2. These two diagrams represent the contributions of the RPA fluctuation and counter term, and can be expressed in the form

\[ \Sigma(i\omega) = \Sigma(1/N')(i\omega) - \lambda + O \left( \frac{1}{N^2} \right) , \]

\[ \Sigma(1/N')(i\omega) = \frac{g \pi \Delta}{N - 1} \int \frac{d\omega'}{2\pi} G_0(i\omega - i\omega') \Pi(i\omega') , \]

where \( N' = N - 1 \). Therefore, from the renormalization condition defined in Eq. (13), the counter term can be deduced to the first order in \( 1/(N-1) \),

\[ \lambda = \Sigma(1/N')(0) - O \left( \frac{1}{N^2} \right) . \]

In a similar way the coefficient \( \lambda_k \) of the counter term can be determined order by order. We can also calculate the leading order term of \( \tilde{\gamma} \) from \( \Sigma(1/N')(i\omega) \),

\[ \tilde{\gamma} = 1 + \frac{K^*}{N - 1} \left[ \frac{K^*}{1 + K^*} + T_S \right] + \tilde{\gamma} \frac{\pi \Delta}{\Delta} \int \frac{d\omega'}{2\pi} [G_0(i\omega')]^2 \Pi(i\omega') . \]

Here, \( \tilde{\gamma} \frac{\pi \Delta}{\Delta} \) denotes the next-leading order contributions, which will be taken into account later.
the right-hand side of Eq. (17), Note that the contributions of the diagrams shown in Fig. 4 vanish at half-filling. This is because the particle-particle and particle-hole pairs give opposite contributions, and cancel each other in the particle-hole symmetric case.

Summing up the contributions from all these diagrams, we calculate the Wilson ratio \( R \), defined in Eq. (9), to order \( 1/(N - 1)^2 \). The result of the renormalized coupling \( \tilde{K} \) can be expressed in the following form, which is exact up to terms of order \( 1/(N - 1) \),

\[
\tilde{K} = \frac{K^*}{1 + K^*} \left[ 1 + \left( \frac{K^*}{N - 1} \right) I_S - \frac{1}{1 + K^*} I_A \right],
\]

\[
I_A = \left[ 1 + \left( E_d^* \right)^2 \right] \frac{\pi \Delta}{2} \int \frac{d\omega}{2\pi} \frac{G_0(i\omega) + G_0(-i\omega)}{1 + g\pi \Delta \chi_0(i\omega)} \right]^2.
\]

In this formula the contribution described by \( I_A \), emerging in the numerator in the right-hand side of Eq. (25), becomes finite in the particle-hole asymmetric case, and it represents the contributions from the eight diagrams in Fig. 4 excluding the first two caused by the counter term. The prefactor \( K^*/(1 + K^*) \) in the right-hand side of Eq. (25) is required to be calculated to order \( 1/(N - 1) \), by including the energy shift due to Eq. (21). Alternatively, through Eq. (14) with Eq. (22), the bare parameter \( \xi_d \) can be determined as a function of \( E_d^* \) to order \( 1/(N - 1) \).

We also consider the next-leading order term of the self-energy, which we found in the previous work gives important contributions to the renormalization factor \( z \) in the particle-hole symmetric case.† The order \( 1/(N - 1)^2 \) self-energy corrections arise from the diagrams shown in Figs. 5 and 6. Furthermore, the corrections arise also from the second and third diagrams in Fig. 2 through the higher-order component of \( \mathcal{U}_{\text{nnb}}(i\omega) \) and that of \( \lambda \), respectively. In the particle-hole asymmetric case, the diagrams indicated in Fig. 5 give finite contributions as the exact cancellation between the particle-particle and particle-hole pairs occurs only at half-filling. We have calculated all these next-leading order contributions of the self-energy numerically to obtain \( \tilde{\gamma}, \lambda, E_d^* \) and the phase shift \( \delta \) to order \( 1/(N - 1)^2 \).

IV. NUMERICAL RESULTS

We have also carried out the NRG calculations for \( N = 4 \), and have compared with the results of the \( 1/(N - 1) \) expansion. We find generally that the next-leading order results agree well with the NRG results, especially for small interactions \( g \lesssim 3.0 \). Typical examples are presented in Figs. 7 and 8.

In Fig. 7 comparisons are made for \( \langle n_{dm} \rangle, \sin^2 \delta \) and \( \xi_d \), choosing a rather large value \( g = 9.0 \) for the interaction in order to show clearly the small deviations. We see the very close agreement between the order \( 1/(N - 1) \) results (red solid line) and the NRG (●) results over the whole region of \( \xi_d \). The order \( 1/(N - 1) \) results, corresponding to the HF-RPA, are also plotted in Fig. 7 with the green dash-dot line although they are almost concealed under the red solid line. Nevertheless, a very small deviation is visible near \( \xi_d^2/(\pi \Delta g) \approx \pm 0.4 \), showing that the order \( 1/(N - 1)^2 \) corrections improve the results slightly closer to the exact NRG results. It indicates that
FIG. 7. (Color online) \(\langle n_{dm}\rangle = \delta/\pi\) and \(\sin^2 \delta\) (upper panel), and \(\xi_d\) (lower panel) plotted as a function of \(\xi_d/(\pi \Delta g)\) for \(N = 4\) and \(g = 9.0\). The circles (●) represent the NRG results, and the red solid line the order 1/\((N - 1)^2\) results. The blue dashed line denotes the zeroth order results obtained without the RPA corrections. The order 1/\((N - 1)\) results, corresponding to the HF-RPA, are also plotted with the green dash-dot line although it is almost concealed under the red solid line.

FIG. 8. (Color online) Renormalized parameters \(\tilde{K}\) (upper panel) and \(z\) (lower panel) plotted as a function of \(\xi_d/(\pi \Delta g)\) for \(N = 4\), choosing \(g = 2.0\) and 9.0. The circles (●) represent the NRG results. The blue dashed line represents the leading order results, corresponding to the HF-RPA. The read solid line represents the next-leading order results, for which the fluctuation beyond the RPA are taken into account.

The phase shift \(\delta\) can be approximated reasonably by the order 1/\((N - 1)\) self-energy given in Eq. (21), which significantly improves the simple HF values (blue dashed line) given at the zeroth order without taking into account the RPA fluctuations. We have also confirmed similar trend for a larger value of the repulsion \(g = 12.0\). We also see in the lower panel of Fig. 7 that the renormalized impurity level \(\bar{\epsilon}_d\) stays close to the Fermi level in the region \(|\xi_d/(\pi \Delta g)| \lesssim 0.3\) as the interaction \(g\) is relatively large in this case. Outside of this region the impurity states tend to be empty at \(\xi_d/(\pi \Delta g) \gtrsim 0.5\), or fully occupied at \(\xi_d/(\pi \Delta g) \lesssim -0.5\). We note that the NRG results for \(\sin^2 \delta\) and \(\langle n_{dm}\rangle\) wave weakly at \(\xi_d/(\pi \Delta g) \simeq \pm 0.3\), relating to the Coulomb oscillation discussed below.

In Fig. 8 the renormalized parameters \(\tilde{K}\) and \(z\) are plotted for \(N = 4\), choosing \(g = 2.0\) and 9.0. We see that the next-leading order corrections (red solid line) significantly improve the leading order results corresponding to the HF-RPA (blue dashed line), towards the exact NRG values (solid circles). Specifically, for small interactions \((g = 2.0)\), the close agreement between the next-leading order results and that of the NRG are seen both for \(\tilde{K}\) and \(z\). However, for large interactions \((g = 9.0)\), the NRG results show an oscillatory behavior, as reported recently also in Ref. 17. This behavior is seen more clearly for the renormalization factor \(z\) than the coupling \(\tilde{K}\). The oscillation is caused by addition of electron into the local orbitals, which in the atomic limit of \(\Delta = 0\) occurs discontinuously at \(-\epsilon_d/U = 0, 1, 2, \ldots, N - 1\). Thus, for strong Coulomb interactions, \(N - 1\) local minima (maxima) appear for \(z (\tilde{K})\) in the region of \(|\xi_d/(\pi \Delta g)| \lesssim 0.5\), which corresponds to \(-(N - 1)U \leq \epsilon_d \leq 0\).

Truncation of the 1/\((N - 1)\) expansion does not reproduce the oscillatory behavior. Nevertheless, we see in Fig. 8 that the next-leading order results of \(\tilde{K}\) are still close to the exact NRG results even for large \(g = 9.0\), especially at the plateau region for \(|\xi_d/(\pi \Delta g)| \lesssim 0.2\), where \(\tilde{K}\) reaches near the unitary-limit value 1.0 and the charge excitation is suppressed significantly. Furthermore, we also see that the order 1/\((N - 1)^2\) results of \(z\) for \(g = 9.0\) approach closely the maxima, emerging at \(\xi_d/(\pi \Delta g) \simeq \pm 0.17\) in the NRG results, which correspond to mixed-valence regions in between two adjacent integer charge states. Therefore, the fluctuations beyond the RPA, taken into account to order 1/\((N - 1)^2\), can describe approximately an upper envelop for the waving curve of the renormalization factor, \(z\), for \(N \geq 4\). Note
that the Kondo energy scale can also be estimated from this result of $z$ as the width of the Kondo resonance is given by $\Delta = z\Delta$.

In order to clarify the dependence of the renormalized parameters on the orbital degeneracy $N$, the next-leading order results of $K$ and $z$ for several values of $N$ (= 4, 6, . . .) are shown in Figs. 9 and 10 for $g$ = 9.0 and 2.0. In these figures, the NRG results for $N = 2$ (orange dash-dot line) and the exact values in the $N \to \infty$ limit (gray dashed line) are also shown. We see, in both strong $g$ = 9.0 and weak $g = 2.0$ coupling cases, the value that the renormalized coupling $\tilde{K}$ can take at $N \geq 4$ is bounded in a narrow region between the curve for $N = 4$ and the one for the large $N$ limit that is described by the RPA given in Eq. (19). As $N$ increases, $\tilde{K}$ converges rapidly to the asymptotic value in the $N \to \infty$ limit.

The zeroth-order HF results for $\langle n_{dm} \rangle$, $\sin^2 \delta$ and $\tilde{\xi}_d$, which are plotted in Fig. 7 with the blue dashed lines, correspond to the exact values in the large $N$ limit. Therefore, as $N$ increases from $N = 4$ to $\infty$, the phase shift $\delta$ and the renormalized impurity level $\tilde{\xi}_d$ vary also in a narrow region between the red-solid and blue-dashed lines indicated in Fig. 4.

In contrast, we see in the lower panel of Figs. 9 and 10 that the renormalization factor $z$ varies in a wider range. Specifically, for large interaction $g = 9.0$, it varies in the range of $0.4 \lesssim z \lesssim 1.0$ at $|\xi_d|/(\pi\Delta g) \lesssim 0.3$ as the orbitals increases from $N = 4$ to $N \to \infty$. As mentioned for Fig. 8, the next-leading order results of $z$ become less accurate than that of $\tilde{K}$ for large $g$. Nevertheless, we also see in Fig. 8 that for small interactions ($g = 2.0$) the order $1/(N - 1)^2$ corrections dominate the fluctuations beyond the RPA, and capture reasonably the correlation effects, especially in the mixed-valence regime.

V. SUMMARY

In summary, we have described the $1/(N - 1)$ expansion approach to the SU($N$) Anderson model with finite Coulomb interaction, without assuming the particle-hole symmetry. We have calculated the renormalized parameters up to order $1/(N - 1)^2$. Specifically, the results of the phase shift $\delta$, or $\tilde{E}_d$, show very close agreement with the NRG results for $N = 4$. This trend has been confirmed for $g \lesssim 10.0$, from small to relatively large interactions. The scaled Wilson ratio $\tilde{K} = (N - 1)/(R - 1)$ and the renormalization factor $z$ also agree well with the exact value in the mixed-valence regime, or not too large.
interactions. As $N$ increases from $N = 4$, $K$ varies in a narrow range and converges rapidly to the RPA value that is asymptotically exact in the large $N$ limit, whereas $z$ varies in a wider range. This behavior of $K$ and $z$ is determined essentially by the fluctuations beyond the HF-RPA, captured through the order $1/(N-1)^2$ corrections.

The $1/(N-1)$ expansion provides a well-defined and controlled way to take into account the fluctuations beyond the HF-RPA. Furthermore, the expansion scheme based on the standard Feynman diagrammatic formalism for fermions with two-body interactions is quite general and flexible. Therefore, this approach has wide potential applications, such as the nonequilibrium problem in the Keldysh formalism and the Hubbard-type lattice models.

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Appendix A: Coefficients for the bubble diagrams

The contribution of the bubble diagram on the vertex correction for $m \neq m'$, shown in Fig. 1, is not a simple geometric series in powers of $U$,

$$U_{\text{bub}}(i\omega) = U + U \sum_{k=1}^{\infty} A_k \left[-U \chi_0(i\omega)\right]^k,$$  \hspace{1cm} (A1)

where $\chi_0(i\omega)$ represents the contribution of a single loop,

$$\chi_0(i\omega) \equiv -\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} G_0(i\omega + i\omega') G_0(i\omega') = \frac{1}{\pi} \frac{\Delta}{|\omega|(|\omega| + 2\Delta)} \log \left[\frac{(|\omega| + \Delta)^2 + E_d^2}{\Delta^2 + E_d^2}\right].$$  \hspace{1cm} (A2)

Specifically, $\pi \Delta \chi_0(0) = 1/[1 + (E_d^4/\Delta^2)]$ in the static limit $\omega \to 0$. The coefficient $A_k$ in Eq. (A1) arises from the summations over the orbital indices for the series of $k$ fermion loops, which can be calculated as

$$A_k = \sum_{m_1}^{'} \sum_{m_2}^{'} \cdots \sum_{m_k}^{'} \prod_{p=0}^{k} \left[\frac{(N-1)^{k+1} - (-1)^{k+1}}{N}\right]$$

$$= \left(\frac{N-1}{N}\right)^k \sum_{p=0}^{k} \left(\frac{-1}{N-1}\right)^p.$$  \hspace{1cm} (A3)

Here, the primed sums for $m_j$'s run under the restriction due to the Pauli exclusion; $m_j \neq m_{j+1}$ for $j = 0, 1, \ldots, k$ with $m_0 = m$ and $m_{k+1} = m'$. Equation (A3) shows that the coefficient $A_k$ can be regarded as a polynomial of $(N-1)$, and $U_{\text{bub}}(i\omega)$ has the higher-order components in the expansion with respect to $1/(N-1)$.