1/(N−1) expansion based on a perturbation theory in U for the Anderson model with N-fold degeneracy

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We study low-energy properties of the N-fold degenerate Anderson model. Using a scaling that takes $u = (N−1)U$ as an independent variable in place of the Coulomb interaction $U$, the perturbation series in $U$ is reorganized as an expansion in powers of $1/(N−1)$. We calculate the renormalized parameters, which characterize the Kondo state, to the next leading order in the $1/(N−1)$ expansion at half-filling. The results, especially the Wilson ratio, agree very closely with the exact numerical renormalization group results at $N = 4$. This ensures the applicability of our approach to $N > 4$, and we present highly reliable results for nonequilibrium Kondo transport through a quantum dot.

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The Anderson impurity has been studied extensively as a model for strongly correlated electrons in dilute magnetic alloys, quantum dots, and also for bulk systems in conjunction with the dynamical mean-field theory [1]. For quantum dots, the nonequilibrium Kondo effect can occur when a bias voltage is applied between two leads. A universal Fermi-liquid behavior [2,3] has been closely examined at low energies for the steady current [6–11] and shot noise [12–17].

Orbital degeneracy in the impurity states also affects the nonequilibrium properties at low energies. Recently, Mora et al. [15] have succeeded to express the current noise in terms of the Fermi-liquid parameters [2,3] in an SU(N) Kondo regime, where the Coulomb repulsion $U$ is so large that charge fluctuations are suppressed near the impurity with N-fold degeneracy. A complementary expression that takes into account the fluctuations at half-filling has been presented in our previous work [18]. In this case, the corrections due to finite $U$ enter through the Wilson ratio $R$, which is a correlation function defined with respect to the equilibrium ground state, and through the width of the Kondo resonance $\Delta$. Therefore, explicit values of these two parameters, $R$ and $\Delta$, are required to study the low-energy transport thoroughly. The exact numerical renormalization group (NRG) approach is still applicable to multi-orbital systems. It practically works, however, for small degeneracies $N < 4$ [18,19], which for $N = 2$ corresponds to the spin degeneracy. Therefore, alternative approaches are needed to explore the large degeneracies at $N > 4$.

In this Letter, we propose a systematic approach to calculate correlation functions at $N > 4$, using a scaling that takes $u = (N−1)U$ as an independent variable in place of $U$. Here, the factor $N−1$ corresponds to the number of different impurity states, with which a local electron in the impurity site can interact. With this scaling, the perturbation series in $U$ can be reorganized as an expansion in powers of $1/(N−1)$, using a diagrammatic classification similar to the one for the N-component $\varphi^4$ model [20]. However, our approach is completely different from the usual $1/N$ expansion and non-crossing approximation, which are constructed on the basis of the perturbation expansion in the hybridization matrix element $v_{\nu}$ [21–23]. We calculate $R$ and $\Delta$ up to the next leading order terms in the $1/(N−1)$ expansion at half-filling, and find that the results agree very closely with the NRG results at $N = 4$, where $N$ is still not so large. Particularly, the Wilson ratio shows an excellent agreement over the whole range of $U$. The early convergence of the expansion implies that our scaling procedure efficiently captures the orbital effects, and ensures the applicability to $N > 4$. This enables us to present highly reliable results for the nonequilibrium steady current and shot noise for $N > 4$. Our approach could have wide application to quantum impurities, and could be used as a solver for the dynamical mean-field theory [24].

The Hamiltonian for the N-fold degenerate Anderson model connected to two leads $(\nu = L, R)$ is given by

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_U, \quad \mathcal{H}_U = \frac{1}{2} \sum_{m \neq m'} U n_{dm} n_{dm'},$$

(1)

$$\mathcal{H}_0 = \sum_{\nu=L,R} \sum_{m=1}^N \int_{-D}^D d\epsilon \epsilon c_{\nu m}^\dagger c_{\nu m} + \sum_{m=1}^N \epsilon_m d^\dagger_m d_m,$$

$$+ \sum_{\nu=L,R} \sum_{m=1}^N \nu \left( d^\dagger_m \psi_{\nu m} + \text{H.c.} \right).$$

(2)

Here, $d^\dagger_m$ creates an electron with energy $\epsilon_m$ in orbital $m$ at the impurity site, $n_{dm} = d^\dagger_m d_m$, and $m = 1, 2, \cdots, N$ includes the spin degrees of freedom. $\epsilon^\dagger_{\nu m}$ creates a conduction electron with energy $\epsilon$ and orbital $m$ in lead $\nu$, and is normalized as $\{c_{\nu m}, \epsilon^\dagger_{\nu m'}\} = \delta_{\nu \nu'} \delta_{mm'} \delta(\epsilon - \epsilon')$. The linear combination $\psi_{\nu m} \equiv \int_{-D}^D d\epsilon \sqrt{\rho} c_{\nu m}$, with $\rho = 1/(2D)$, couples to the impurity level via the hybridization matrix element $v_{\nu}$, and $\Delta = \Gamma_L + \Gamma_R$ with
\( \Gamma_{\nu} = \pi \rho \nu^2 \). We consider the parameter region where \( \Delta, \epsilon_d, \) and \( U \) are much smaller than the half band width \( D \).

We use the imaginary-frequency Green’s function that takes the form \( G(i\omega) = [(i\omega - \epsilon_{d} + i\Delta \text{sgn} \omega - \Sigma(i\omega))]^{-1} \) for \( |\omega| \ll D \). The behavior of the self-energy \( \Sigma(i\omega) \) for small \( \omega \) determines the enhancement factor for the linear specific heat \( \bar{\gamma} = 1 - \partial \Sigma(i\omega)/\partial(i\omega)|_{\omega=0} \) and the renormalized parameters \( z = 1/\bar{\gamma}, \epsilon_{d} = z(\epsilon_{d} + \Sigma(0)) \), and \( \Delta = z\Delta \). The average number of local electrons can be deduced from the phase shift \( \delta \coloneqq \cot^{-1}(\bar{\gamma} z/\Delta) \), using the Friedel sum rule, \( \langle n_{dm} \rangle = \Omega/\pi \). The enhancement factor for the spin susceptibility and that for the \( \chi \) vertex function \( \Gamma \) can be deduced from the self-energy and four-point diagrammatic representation of the perturbation in \( \bar{\gamma} \) appears at \( N \) degeneracy [4]. For \( \epsilon_{d} \) takes the form \( \tilde{\chi}_{m} \equiv \chi_{mm} - \chi_{mm'} \) and \( \tilde{\chi}_{c} \equiv \chi_{mm} + (N-1) \chi_{mm'} \) for \( m \neq m' \). These susceptibilities can be deduced from the self-energy and four-point vertex function \( \Gamma_{mm';mm'}(i\omega_{1}, i\omega_{2}; i\omega_{3}, i\omega_{4}) \) for \( m \neq m' \), using the Ward identities [5].

\[
\tilde{\chi}_{mm} = \bar{\gamma}, \quad \tilde{\chi}_{mm'} = -\frac{\sin^{2} \delta}{\pi \Delta} \Gamma_{mm';mm'}(0,0;0,0). \tag{3}
\]

Furthermore, \( \bar{U} \equiv z^{2} \Gamma_{mm';mm'}(0,0;0,0) \) corresponds to the residual interaction between the quasi-particles.

The Wilson ratio \( R \) parameterizes how far the system is away from the Kondo limit, and plays a central role for finite \( U \),

\[
R \equiv \frac{\tilde{\chi}_{c}}{\bar{\gamma}} = 1 + \frac{\bar{g}}{N-1} \sin^{2} \delta, \quad \tilde{\chi}_{c} = 1 - \bar{g} \sin^{2} \delta. \tag{4}
\]

Here, the scaling factor \( N-1 \) is introduced to the renormalized interaction \( \bar{U} \) and the bare one \( U \), such that

\[
\tilde{g} \equiv (N-1) \frac{\bar{U}}{\pi \Delta}, \quad g \equiv (N-1) \frac{U}{\pi \Delta}. \tag{5}
\]

In the following we consider the particle-hole symmetric case, where \( \epsilon_{d} = -(N-1)U/2 \) and \( \delta = \pi/2 \). In this case, the renormalized coupling takes a value in the range \( 0 \leq \tilde{g} \leq 1 \). It approaches to \( \tilde{g} \rightarrow 1 \) in the limit of \( g \rightarrow \infty \) as the charge fluctuation is suppressed \( \tilde{\chi}_{c} \rightarrow 0 \).

We calculate \( \bar{\gamma} \) and \( \Gamma_{mm';mm'}(0,0;0,0) \) perturbatively to order \( U^{3} \) and \( U^{4} \), respectively, by extending Yamada’s calculations for \( N = 2 \) to general \( N \) [18], and obtain the leading order contributions in the \( 1/N \) limit are given by

\[
\tilde{\gamma} = 1 + \frac{1}{N-1} \left[ \left( 3 - \frac{\pi^{2}}{4} \right) \bar{g}^{2} - \left( \frac{21}{2} \zeta(3) - 7 - \frac{\pi^{2}}{2} \right) \frac{N-2}{N-1} \bar{g}^{3} + O(\bar{g}^{4}) \right]. \tag{7}
\]

Here, \( \zeta(x) \) is the Riemann zeta function, which disappears at \( N = 2 \) where the impurity has only the spin degeneracy [4]. For \( N > 2 \), \( \bar{\gamma} \) and \( \bar{g} \) are no longer even nor odd function of \( U \). We see in Eqs. (6) and (7) that the coefficients in the perturbation series can be expanded in powers of \( 1/(N-1) \). Thus, the perturbation series in \( g \) can be reorganized as an expansion with respect to \( 1/(N-1) \). If the \( N \rightarrow \infty \) limit is taken at fixed \( g \), then the right hand side of Eq. (6) approaches to an alternating geometric series in \( g \), and \( \bar{\gamma} \) approaches to the noninteracting value \( \bar{\gamma} \rightarrow 1 \). We will see later that these are true for all order in \( g \), and the asymptotic forms of Eqs. (6) and (7) in the large \( N \) limit are given by

\[
\tilde{\gamma} = \frac{g}{1+g} + O\left(\frac{1}{N-1}\right), \quad \bar{\gamma} = 1 + O\left(\frac{1}{N-1}\right). \tag{8}
\]

The corrections due to finite \( N \) can be extracted, using a diagrammatic representation of the perturbation in \( U \).

The leading order contributions in the \( 1/(N-1) \) expansion arise form a series of the bubble diagrams indicated in Fig. 1 and the sum of these diagrams corresponds to

\[
U_{\text{bab}}(i\omega) = \frac{\phi(i\omega)}{N-1} + \frac{g\pi \Delta \Pi(i\omega)}{(N-1)^2} + O\left(\frac{1}{(N-1)^3}\right), \tag{9}
\]

\[
\phi(i\omega) \equiv \frac{g\pi \Delta}{1 + g\pi \Delta \chi_{0}(i\omega)}. \quad \Pi(i\omega) \equiv \chi_{0}(i\omega) \phi(i\omega). \tag{10}
\]

Here, \( \chi_{0}(i\omega) \equiv - \int \frac{d\omega'}{2\pi} G_{0}(i\omega + i\omega')G_{0}(i\omega') \), and \( G_{0}(i\omega) = [i\omega - E_{d} + i\Delta \text{sgn} \omega]^{-1} \) with \( E_{d} = 0 \) [23]. Thus \( \chi_{0}(i\omega) = \frac{1}{\pi \Delta} \frac{\log(1+|i\omega|)}{|i\omega|} \) with \( x = \omega/\Delta \). The propagator \( U_{\text{bab}}(i\omega) \) contains not only the leading order, but also higher order contributions in the \( 1/(N-1) \) expansion. This is because the orbital indices for adjacent bubbles have to be different, and summations over internal \( m \)'s are not independent. The order \( 1/(N-1) \) contributions to the vertex and self-energy come from the diagrams shown in Fig. 2.

To calculate the renormalized coupling constant \( \tilde{g} \) to order \( 1/(N-1) \), we need \( \Gamma_{mm';mm'}(0,0;0,0) \) to order \( 1/(N-1)^{2} \) as \( \tilde{g} \) has a scaling factor \( N-1 \) defined in Eq.
The order $1/(N - 1)^2$ contributions to the vertex function arise from the diagrams shown in Fig. 3, and from the order $1/(N - 1)$ component of the vertex diagram in Fig. 2. Summing up all these contributions, $\tilde{g}$ can be expressed in the form that is exact up to terms of order $1/(N - 1)$,

$$\tilde{g} = \frac{g}{1 + g} \left[ 1 + \frac{2g}{1 + g} \right] \frac{\mathcal{I}_φ(g)}{1 + \frac{g^2}{1 + g} \mathcal{I}_φ(g)} + O\left(\frac{1}{N^2}\right).$$  \hspace{1cm} (11)$$

Here, $\mathcal{I}_φ(g) = \mp \Delta \int \frac{d\omega}{2\pi} \{G_φ(i\omega)\}^2 \Pi(i\omega)$, and $N' = N - 1$. This formula shows the correct asymptotic form in both the weak and the strong coupling limits: $\tilde{g} \simeq g$ for $g \to 0$, and $\tilde{g} \to 1$ for $g \to \infty$. Thus, Eq. (11) can also be regarded as an interpolation formula for the Wilson ratio as $R - 1 = \tilde{g}/(N - 1)$ at half-filling. The order $1/(N - 1)$ results for $\tilde{g}$ show an excellent agreement with the NRG results for $N = 4$ as indicated in Fig. 5 (a).

To obtain Eq. (11), the parameter $\tilde{g}$ in the denominator has been taken into account up to order $1/(N - 1)$,

$$\tilde{g} = 1 + \frac{g}{N - 1} \left[ \frac{g}{1 + g} + \mathcal{I}_φ(g) \right] + \tilde{g}'(\frac{1}{N^2}) + O\left(\frac{1}{N^3}\right).$$  \hspace{1cm} (12)$$

We also calculate, $\tilde{g}'(\frac{1}{N^2})$, the order $1/(N - 1)^2$ contributions which arise from the diagrams shown in Fig. 4 and from the higher order component of the self-energy diagram in Fig. 2.

Figure 3 (a) shows a comparison between the NRG and the $1/(N - 1)$ expansion results for $N = 4$. We see the very close agreement, especially for $g$. Although the order $1/(N - 1)$ results are slightly smaller than the NRG results, the two curves for $\tilde{g}$ almost overlap each other over the whole range of $g$. The deviation must decrease as $N$ increases. Therefore, the order $1/(N - 1)$ formula for $\tilde{g}$ given in Eq. (11) provides almost exact numerical values for $N > 4$. We also see in Fig. 5 (b) the value that $\tilde{g}$ can take is bounded in a very narrow region between the curve for $N = 4$ and that for the $N \to \infty$ limit. As $N$ increases, $\tilde{g}$ varies rapidly towards the value for the large $N$ limit. The order $1/(N - 1)^2$ results for the renormalization factor $z$, shown in Fig. 5 (a), also agree with the NRG results for $N = 4$ at $g^2 \lesssim 3.0$, or equivalently $\tilde{g} \lesssim 0.8$, from the weak to the intermediate coupling region where $\tilde{g}$ is still not converged to 1.0, the value for the strong coupling limit. Therefore, away from the strong coupling regime the Kondo energy scale, $\Delta = z\Delta$, can be deduced reasonably from the order $1/(N - 1)^2$ results.

The $1/(N - 1)$ expansion can be applied fruitfully to nonequilibrium transport at finite $U$. To be specific, we choose the lead-dot couplings and chemical potentials to be symmetric: $G_L = G_R$ and $\mu_L = -\mu_R = (eV/2)$. In this case, an exact expression can be derived for the retarded Green’s function at low energies up to order $\omega^2$, $T^2$, and $(eV)^2$ (3) (a),

$$G^r(\omega) \simeq \frac{z}{\omega + i\Delta + i\frac{\tilde{g}^2}{2(N - 1)\Delta}} \left[ \omega^2 + \frac{\tilde{g}^2}{2}(eV)^2 + (\pi T)^2 \right].$$  \hspace{1cm} (13)$$

The differential conductance for the current through the impurity can be deduced from $G^r(\omega)$, using the formula by Meir-Wingreen (20) and Hershfield (21),

$$\frac{dJ}{dV} = \frac{Ne^2}{h} \left[ 1 - c_T \left( \frac{\pi T}{\Delta} \right)^2 - c_V \left( \frac{eV}{\Delta} \right)^2 + \cdots \right],$$  \hspace{1cm} (14)$$

$$c_T = \frac{1}{3} \left( 1 + \frac{2\tilde{g}^2}{N - 1} \right), \hspace{1cm} c_V = \frac{1}{4} \left( 1 + \frac{5\tilde{g}^2}{N - 1} \right).$$  \hspace{1cm} (15)$$

The low-energy behavior is characterized by the two parameters, $\tilde{g}$ in the coefficients and $\Delta$ the energy scale,
which depend on \( N \). Figure 5(a) shows the ratio of \( c_T \) to \( c_V \) as a function of \( g \) for several \( N \), using Eq. (11) for \( N \geq 6 \). The ratio takes a value in the range \( 3/4 \leq c_T/c_V \leq (3/4)(N+4)/(N+1) \) [28]. The order \( 1/(N-1) \) results for \( g \) are numerically almost exact for \( N > 4 \) as mentioned, and thus the results shown in Fig. 5(a) capture orbital effects correctly.

As another application of Eq. (11), we also consider the shot noise \( S = \int dt \left[ \langle \delta \hat{J}(t) \delta \hat{J}(0) \rangle / 2 \right] \) for the symmetric Anderson model for \( N = 2 \) [13, 17], and for general \( N \):

\[
S = \frac{N - 1}{N} \left( 1 + \frac{g^2}{N} \right) \left( \frac{N}{2} \right)^2 eV \quad (18) \]

The Fano factor \( F_b \) is defined as the ratio of \( S \) to the backscattering current \( J_b = NeV/\hbar - J \), and has been obtained in the form [18],

\[
F_b = \frac{S}{2eJ_b} = 1 + \frac{g^2}{N} + \frac{5g^2}{N-1}. \tag{16}
\]

It takes a value in the range \( 1 \leq F_b \leq (N+8)/(N+4) \). In Fig. 5(b), the order \( 1/(N-1) \) results for \( F_b \) are plotted as functions of \( g \) for \( N \geq 6 \), together with the exact results for \( N \leq 4 \) [15]. As \( N \) increases, \( \tilde{g} \) converges rapidly to the value, \( \tilde{g} \approx g/(1+g) \), for the large \( N \) limit, as mentioned in the above. Thus, for \( N \gtrsim 8 \), the dependence is determined essentially by the factor \( 1/(N-1) \), seen explicitly in Eq. (16). The \( 1/(N-1) \) expansion can also be applied to the full counting statistics [21].

In conclusion, we have described the \( 1/(N-1) \) expansion approach based on the scaling defined in Eq. (19). The next leading order results for \( \tilde{g} \), which at half-filling corresponds to \( \tilde{g} = (N-1)/(R-1) \), can be expressed in the form of Eq. (11). We find that this formula interpolates almost exactly between the weak and the strong coupling limits for \( N \geq 4 \). The \( 1/(N-1) \) expansion can be extended to explore the particle-hole asymmetric case [22]. Furthermore, it provides a well-defined and controlled way to take into account the fluctuations near the \( N \to \infty \) fixed point of many fermion systems with two-body interactions.

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\[\text{FIG. 5. (Color online) (a): } \tilde{g} \text{ and } z \text{ versus } g \text{ for } N = 4 \text{. The curve with the circles represents the NRG results. The red dotted line represents the order } 1/(N-1) \text{ results for } \tilde{g}, \text{ and the blue dashed line the order } 1/(N-1)^2 \text{ results for } z. \text{ (b): } \tilde{g} \text{ vs } g \text{ for } N = 2 \text{ (Bethe ansats)} [4], N = 4 \text{ (NRG)}, N = 6 \text{ (order } 1/(N-1)\text{)}, \text{ and for } N \to \infty \text{ where } \tilde{g} \to g/(1+g).\]

\[\text{FIG. 6. (Color online) Plots of (a) } c_v/c_T \text{ and (b) } F_b \text{ as a function of } g \text{ for } N = 2 \text{ (Bethe ansats)}, N = 4 \text{ (NRG), and for } N \geq 6 \text{ the order } 1/(N-1) \text{ results. In the } N \to \infty \text{ limit, the curves approach to (a) } c_v/c_T \to 3/4 \text{ and (b) } F_b \to 1.\]

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