# Exact perturbative solution of the Wolff model with electron-hole symmetry

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(Received 9 March 1989)

The spin and charge susceptibilities of the Wolff model with electron-hole symmetry and the Lorentzian density of band states are obtained exactly by standard perturbation theory. The solution is valid for any value of the Coulomb interaction and exhibits features which are observed experimentally in some strongly-interacting-fermion systems.

The presence of local Coulomb correlations in metallic systems gives rise to many remarkable phenomena like the Kondo effect,[1] valence fluctuations,[2] heavy fermions,[3] high-temperature superconductivity,[4] etc. Although different in detail and described by different models, all these phenomena seem to appear when the on-site Coulomb repulsion $U$ becomes the largest relevant energy parameter. That would suggest that theoretical treatments of strongly interacting fermions, the common name associated with the above-mentioned systems, should start from the large-$U$ limit of the appropriate models. Unfortunately, although easy to formulate, such a program encounters many difficulties.[5] For example, the obvious metallic character of strongly interacting systems becomes a nontrivial property to obtain theoretically.

Surprisingly enough, a qualitative description of many of the phenomena observed with strongly interacting fermions can also be obtained by perturbation theory, starting from the normal metallic state and treating $U$ as an expansion parameter. The low-order expansions seem to reproduce many of the experimentally observed features[6] and even allow one to discuss the small-$U$–large-$U$ transition, which is an essential feature of the models describing strongly interacting fermions. Furthermore, there are nontrivial examples for which the $U$ expansion provides the exact solution.[7–9] Experimentally, despite all the peculiarities the data might display, one seems to be dealing with metallic systems. All this, and the reasons of simplicity, would recommend the perturbation theory as a useful approach to strongly interacting fermions. However, one should mention that the basic question regarding the applicability of the perturbative approach to strongly interacting fermions, i.e., the existence of the normal Fermi-liquid ground state, has no definite theoretical answer even for the most often used models like the Hubbard or the periodic Anderson model.

In this Brief Report we show that the $U$ expansion can be used to obtain the exact solution for the spin and charge susceptibilities of the Wolff model, a particular model of strongly interacting fermions. The results are valid for any value of $U$ and agree with the predictions obtained by the numerical renormalization group method.[10] The paper is organized as follows. First, we define the model, next, formulate the perturbation expansion for the susceptibilities and, finally, derive the exact results.

The Wolff[11] or spin-fluctuation[12] model has been used to discuss the properties of some transition-metal-based alloys[13] (e.g., Rh Fe, Ir Fe, etc.) and some heavy fermions[14] (e.g., $UPt_3$). In these systems, the Kondo anomalies appear in the thermodynamic data, but the electric resistance does not show the typical Kondo minimum (or maximum in heavy-fermion intermetallics). Rather, the electric resistance increases monotonically, albeit very fast, with the increase of temperature. The enhanced magnetic susceptibility, specific heat, and the negative magnetoresistance indicate that the anomalies are due to the presence of large Coulomb correlations at the "magnetic" sites.

The model Hamiltonian is given by

$$H=\sum_{i,j,\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\varepsilon_0\sum_{\sigma}c_{0\sigma}^{\dagger}c_{0\sigma}+Uc_{0\uparrow}^{\dagger}c_{0\uparrow}c_{0\downarrow}^{\dagger}c_{0\downarrow} . \quad (1)$$

The first term in Eq. (1) characterizes the host conduction band in which the on-site Coulomb correlations are neglected. The hopping matrix elements $t_{ij}=t(\mathbf{R}_i-\mathbf{R}_j)$ connect different sites and are assumed to remain unchanged upon alloying. The second and the third term in (1), characterizing the impurity placed at site 0, lead to the potential scattering, proportional to $\varepsilon_0$, and to the many-body effects, due to the on-site Coulomb repulsion $U$. The difference with respect to the Anderson model appears because the symmetry of the relevant "magnetic" impurity states and "nonmagnetic" host states is assumed to be the same. The parameter space for the Wolff model can be defined by dimensionless quantities $\eta$ and $u$, where $\eta=\frac{1}{2}+\varepsilon_0/U$ measures the deviation from the electron-hole symmetry and $u=U/\pi D$ measures the strength of the Coulomb interaction. Here, $D$ is the characteristic energy of the unperturbed conduction band.

The perturbation expansion is formulated above the nonmagnetic mean-field state so that the Hamiltonian is rewritten as $H=H_{\mathrm{HF}}+H'$, where $H_{\mathrm{HF}}$ is the Hartree-Fock approximation of $H$ and

$$H'=U(c_{0\uparrow}^{\dagger}c_{0\uparrow}-\langle n_{0\sigma}\rangle_{\mathrm{HF}})(c_{0\downarrow}^{\dagger}c_{0\downarrow}-\langle n_{0\sigma}\rangle_{\mathrm{HF}}) . \quad (2)$$

 

To obtain the expressions for the spin and charge susceptibilities, $\chi_s$ and $\chi_c$, one adds the appropriate conjugate fields to $H'$ and evaluates the second derivative of the free energy with respect to those fields. The standard $S$-matrix expansion generates the power series for $\chi_s' \equiv [2\pi D/(g\mu_B)^2]\chi_s$ and $\chi_c' \equiv \frac{1}{2}\pi D\chi_c$, with $u = U/\pi D$ as the expansion parameter. Thus, we obtain for the dimensionless quantities $\chi_s'$ and $\chi_c'$ the result

$$\chi_s' = \sum_{n=0}^{\infty} c_n^- u^n \tag{3}$$

and

$$\chi_c' = \sum_{n=0}^{\infty} c_n^+ u^n , \tag{4}$$

where the expansion coefficients are given by

$$c_n^{\pm} = (-1)^n \frac{(\pi D)^{n+1}}{n!\beta} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_{n+2} [D_\uparrow^{n+2}(\tau_1, \ldots, \tau_{n+2}) D_\downarrow^n(\tau_2, \ldots, \tau_{n+1}) \pm D_\uparrow^{n+1}(\tau_1, \ldots, \tau_{n+1}) D_\downarrow^{n+1}(\tau_2, \ldots, \tau_{n+2})]_{\text{con}} \tag{5}$$

and $D_\sigma^n(\tau_1, \ldots, \tau_n)$ are defined as the $n$th-order determinants constructed from the local Hartree-Fock Green's functions, $G_{00}^{0\sigma}(\tau_i - \tau_j)$, with zeros on the main diagonal:

$$D_\sigma^n(\tau_1, \ldots, \tau_n) = \det[(1-\delta_{ij}) G_{00}^{0\sigma}(\tau_i - \tau_j)] . \tag{6}$$

The Fourier transformation of $G_{00}^{0\sigma}(\tau)$ leads to the standard diagrammatic expansion in which the unperturbed propagators, $G_{00}^{0\sigma}(z)$, are given by

$$G_{00}^{0\sigma}(z) = \{[g_{00}^\sigma(z)]^{-1} - E_0^\sigma\}^{-1} . \tag{7}$$

Here, $E_0^\sigma = \varepsilon_0 + \langle n_{0\sigma} \rangle_{\text{HF}} U$, and $g_{00}^\sigma = g_{jj}^\sigma$ is the local Green's function in the absence of the impurities. In the thermodynamic limit it reads

$$g_{jj}^\sigma(z) = \frac{1}{N} \int_{-\infty}^{\infty} \frac{\rho_\sigma^{(0)}(\varepsilon)}{z - \varepsilon} d\varepsilon , \tag{8}$$

where $\rho_\sigma^{(0)}(\varepsilon)$ is the density of the unperturbed host states.

From the structure of the expansion it is clear that any quantity calculated perturbatively for the Wolff model assumes the same form as the corresponding perturbative result for the Anderson model and that all the general identities derived for the Anderson model,[6,15] retain their validity for the Wolff model as well. For example, the linear specific-heat coefficient is given by

$$\gamma' \equiv (3D/2\pi k_B^2)\gamma = \tfrac{1}{2}(\chi_s' + \chi_c') .$$

To proceed, one has to make explicit assumptions about the shape of $\rho_\sigma^{(0)}(\varepsilon)$, and here we take

$$\rho_\sigma^{(0)}(\varepsilon) = \frac{ND}{\pi(\varepsilon^2 + D^2)} , \tag{9}$$

which leads to the result

$$G_{00}^{0\sigma}(z) = [z - E_0^\sigma + iD \operatorname{sgn}(\operatorname{Im} z)]^{-1} . \tag{10}$$

Thus, for the case of the Lorentzian density of unperturbed band states, all the perturbative results for the Wolff model, obtained in the site representation, are the same as the corresponding perturbative expressions for the Anderson model with the rectangular density of unperturbed band states, provided the parameters $E_{d\sigma}$ and $\Delta$ of the Anderson model are replaced by $E_0^\sigma$ and $D$ for the Wolff model.

In general, the coefficients $c_n^\pm = c_n^\pm(E_0^\sigma/D, k_B T/D)$ can be calculated to finite order only and the analysis of the model properties along these lines will be given elsewhere. Here, we note only that the analogy between the Wolff and the Anderson model allows the conclusion that in the large-$u$ limit either the Kondo or the valence-fluctuation features will be obtained, depending on the value of the asymmetry parameter.

In the particular case of the model with the electron-hole symmetry, $E_0^\sigma = 0$, and for $T = 0$, the solution which is valid to all orders in $U$ can be obtained. The coefficients $c_n^\pm$, evaluated with $G_{00}^{0\sigma}$ given by Eq. (10), are known to all orders and it follows[7,8] that $\chi_s'$ and $\chi_c'$ are given by

$$\chi_s' = e^{\pi^2 u/8} \varphi(u) , \tag{11}$$

$$\chi_c'(u) = \chi_s'(-u) , \tag{12}$$

where

$$\varphi(u) = \sum_{n=0}^{\infty} (-1)^n a_n u^n . \tag{13}$$

The coefficients $a_n$ obey the recursive formula

$$a_n = [(\tfrac{1}{8}\pi^2)^n/n!] - (2n-1)a_{n-1} \tag{14}$$

for $n \geq 1$, with $a_0 = 1$, and have the limiting properties $a_n \to 0$ and $|a_{n+1}/a_n| \to 0$ for $n \to \infty$. Thus, $\varphi(u)$ defined by the series expansion (13) is a well-defined function for any value of $u$ and so are $\chi_s'(u)$ and $\chi_c'(u)$.

The function $\varphi(u)$ has a completely different behavior in the small- and large-$u$ limits, which are given by

$$\varphi_{(1)}(u) = 1 - (\tfrac{1}{8}\pi^2 - 1)u \quad \text{as } u \to 0 \tag{15}$$

and

$$\varphi_a(u) = \sqrt{\pi/2u}\, e^{-1/2u} \quad \text{as } u \to \infty . \tag{16}$$

This is illustrated in Fig. 1 where $\varphi(u)$ is plotted together with its asymptotic, large-$u$ form $\varphi_a(u)$ and its first-order and second-order approximations, $\varphi_{(1)}(u)$ and $\varphi_{(2)}(u)$. Note that the transition from small-$u$ to large-$u$ behavior takes place already around $u = 1$. Furthermore, the small-$u$ result, which would be obtained by the finite-order perturbation theory, retains its validity at those values of $u$ for which the exact result is already close to

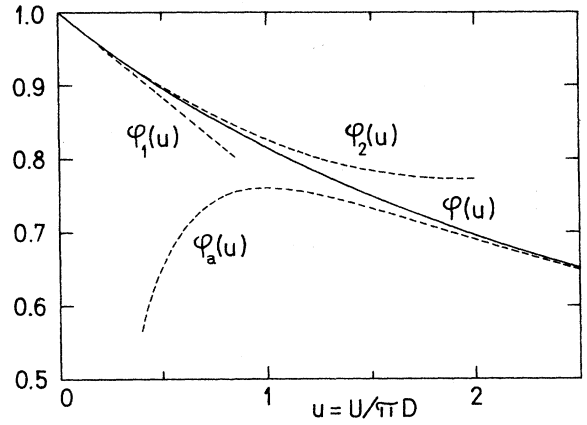


FIG. 1. Function $\varphi(u)$, defined by Eq. (13), together with its asymptotic, large-$u$ form $\varphi_a(u)$ and its first-order and second-order approximations, $\varphi_{(1)}(u)$ and $\varphi_{(2)}(u)$.

the asymptotic $u \to \infty$ result. This is due to the extremely quick convergence of the series (13) which defines $\varphi(u)$: for the first four coefficients one has $a_0=1$, $a_1=0.2337$, $a_2=0.0599$, $a_3=0.0134$, and for $n \gg 1$ they diminish as $a_{n+1}/a_n \leq (\pi^2/8)/(n+2)$. Thus it seems that the finite-order $u$ expansion reproduces, to arbitrary accuracy, even those properties of the model which, at first sight, could be obtained only by studying the large-$u$ limit.

Next, we notice that the self-energy expansion and the expression for the conduction-electrons' $T$ matrix allow the conclusion that the electric resistance of the Wolff model will increase monotonically with temperature and that at low temperatures the power law will be obtained, with the $T^2$ coefficient being inversely proportional to the square of the spin susceptibility. If the Kondo temperature is defined as $k_B T_K/D = 1/\chi_s'(T=0)$, the transport and thermodynamic functions of the model obey, for the physically relevant values of parameters, the scaling laws, as is also the case for the Anderson model. Thus, qualitatively at least, the model exhibits the properties which are experimentally observed in the transition-metal-based dilute alloys and some heavy-fermion systems above the coherence temperature.

In summary, the properties of the Wolff model, which describes particular strongly-interacting-fermion systems, can be obtained by the perturbation theory. The exact solution for the spin and charge susceptibilities, at $T=0$, is obtained analytically for the case with the electron-hole symmetry and the Lorentzian density of band states. In the asymmetric case, the low-order perturbation theory still allows one to discuss the large-$u$ limit in which the scaling laws hold. In that limit the phase diagram of the model comprises the Kondo region ($\eta \approx 0$), the valence-fluctuation region ($\eta \approx \frac{1}{2}$), and the "nonmagnetic region," in which the many-body effects are not pronounced. The numerical analysis of the perturbative results valid for arbitrary asymmetry and for various densities of band states, i.e., the study of the changes in the model properties caused by the interplay between the correlation effects and the band-structure effects, will be discussed elsewhere.

*A note added:* The single-impurity Anderson model proved to be very useful for the understanding of the periodic Anderson model. Likewise, we believe that the solution of the Wolff model might contribute to our understanding of the "periodic Wolff model," that is, the Hubbard model.

Discussions with P. W. Anderson are gratefully acknowledged. This work has been partially supported by the YU-U.S.A. Grants No. JFP-707 and JFP-817-31.

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