Series expansion for the symmetric Anderson Hamiltonian

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Spin susceptibility, charge susceptibility, and specific heat for the symmetric Anderson model can be expanded in power series which converge absolutely for any finite value of the expansion parameter $U/\pi\Delta$. The coefficients of these expansions satisfy the simple recursion relation $C_n=(2n-1)C_{n-1}-(\pi/2)^2\ C_{n-2}$. The expansions rapidly assume their asymptotic form and the scaling behavior is obtained for $U/\pi\Delta \gtrsim 2$.

In this paper we show that the exact results for the symmetric Anderson Hamiltonian,[1] obtained by the Bethe-ansatz method,[2–5] can be represented by convergent power-series expansions in terms of $u=U/\pi\Delta$, irrespective of the magnitude of the expansion parameter, and that the same series expansions could also be generated by the perturbative approach of Yosida and Yamada.[6,7]

The remarkable property of these series expansions is that they rapidly attain the asymptotic form so that the scaling behavior is obtained as soon as the expansion parameter becomes larger than 2. Furthermore, the coefficients in these expansions decrease very fast with increasing order, so that only a limited number of terms suffices for an accurate description of the system, even for $U/\pi\Delta$ as large as 2 or 3, that is, even in the strong correlation regime.

The symmetric nondegenerate Anderson model is defined by the Hamiltonian

$$H=\sum_{k,\sigma}\epsilon_k n_{k\sigma}+\epsilon_d\sum_{\sigma}n_{d\sigma}+V\sum_{k,\sigma}(c_{k\sigma}^{\dagger}c_{d\sigma}+c_{d\sigma}^{\dagger}c_{k\sigma})+Un_{d\uparrow}n_{d\downarrow}\ ,$$

where all symbols have their usual meaning and where $\epsilon_d=-\frac{1}{2}U$. In the weak correlation regime ($U\ll\Delta$) the properties of the model could be simply obtained[8] by a straightforward application of the perturbation theory around the $U=0$ ground state. In the strong correlation regime ($U\gg\Delta$) the behavior of the system is characterized by the scaling laws, and it has been argued that such a behavior could not be obtained by means of the perturbation theory in terms of u.

Since several papers[2–5] regarding the application of the Bethe-ansatz method to the Anderson model have appeared recently, we quote here just the results for the zero-temperature reduced spin susceptibility $\widetilde{\chi}_s=[2\pi\Delta/(g\mu_B)^2]\chi_s$, charge susceptibility $\widetilde{\chi}_c=\frac{1}{2}\pi\Delta\chi_c$, and linear coefficient of the specific heat $\widetilde{\gamma}=(3\Delta/2\pi k_B^2)\gamma$ as follows:

$$\widetilde{\chi}_s=\sqrt{\pi/2u}\ \exp[\tfrac{1}{8}\pi^2u-(1/2u)]+\frac{1}{\sqrt{2\pi u}}\int_{-\infty}^{\infty}\frac{e^{-x^2/2u}dx}{1+(\frac{1}{2}\pi u+ix)^2}\ , \tag{1}$$

$$\widetilde{\chi}_c=\frac{1}{\sqrt{2\pi u}}\int_{-\infty}^{\infty}\frac{e^{-x^2/2u}dx}{1+(\frac{1}{2}\pi u+x)^2}\ , \tag{2}$$

$$\widetilde{\gamma}=\tfrac{1}{2}(\widetilde{\chi}_s+\widetilde{\chi}_c)\ . \tag{3}$$

The exponential term in the expression for $\widetilde{\chi}_s$, which we denote by $E(u)$, has an essential singularity at $u=0$, and it tends to the Kondo susceptibility $\widetilde{\chi}_K=\sqrt{\pi/2u}\ \exp(\frac{1}{8}\pi^2u)$ as $u\rightarrow\infty$. However, before making any conclusions regarding the analytic behavior of the complete spin susceptibility, one should carefully evaluate the exponential corrections to the main value of the integral $I_s=\widetilde{\chi}_s-E$. Rewriting the integral I_s in the form

$$I_s(u)=\frac{1}{\sqrt{2\pi u}}\mathrm{Re}\int_{-\infty}^{\infty}\frac{e^{-x^2/2u}}{x-z'}dx\ , \tag{4}$$

where $z'=-1+i\frac{1}{2}\pi u$, and integrating along the closed contour shown in Fig. 1 we obtain

$$I_s(u)=e^{\pi^2u/8}\sqrt{2/\pi u}\int_0^{\infty}e^{-x^2/2u}\frac{\cos(\frac{1}{2}\pi x)}{1-x^2}dx-E(u)\ , \tag{5}$$

so that "anomalous" exponential term $E(u)$ disappears from the expression (1) for $\widetilde{\chi}_s$ and the remaining integral can be evaluated exactly. Expression (2) for $\widetilde{\chi}_c$ can also be transformed into a more convenient form,

$$\widetilde{\chi}_c(u)=e^{-\pi^2u/8}\sqrt{2/\pi u}\int_0^{\infty}e^{-x^2/2u}\frac{\cosh(\frac{1}{2}\pi x)}{1+x^2}dx\ , \tag{6}$$

by simply shifting the variable of integration by $\frac{1}{2}\pi u$.

In order to calculate the integrals in (5) and (6) we ex-

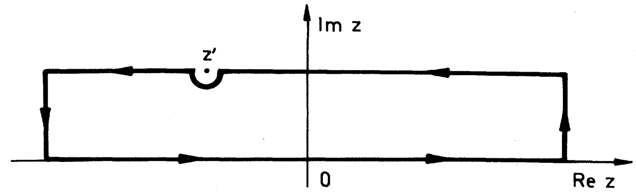

FIG. 1. Closed contour in the complex plane used to evaluate the integral in Eq. (4). The contributions of vertical segments vanish as $|\mathrm{Re}\,z|\rightarrow\infty$.

pand $\cos(\frac{1}{2}\pi x)/(1-x^2)$ and $\cosh(\frac{1}{2}\pi x)/(1+x^2)$ into power series that converge absolutely and uniformly for any $|x| < \infty$; integrating term by term, we obtain

$$\tilde{\chi}_s(u)=\exp(\tfrac{1}{8}\pi^2 u)\varphi(u)\ , \tag{7}$$

$$\tilde{\chi}_c(u)=\exp(-\tfrac{1}{8}\pi^2 u)\varphi(-u)\ , \tag{8}$$

where $\varphi(u)$ denotes the power series

$$\varphi(u)=\sum_{n=0}^{\infty}(-1)^n \zeta_n u^n\ . \tag{9}$$

The coefficients ζ_n are given by

$$\zeta_n=\frac{(\frac{1}{8}\pi^2)^{n+1}}{(2n+1)(n+1)!}\sum_{k=0}^{\infty}(-1)^k\frac{[2(n+1)]!}{[2(n+k+1)]!}\left[\frac{\pi}{2}\right]^{2k} \tag{10}$$

and satisfy the recursion relation

$$\zeta_n=[(\tfrac{1}{8}\pi^2)^n/n!]-(2n-1)\zeta_{n-1} \tag{11}$$

for $n\geq 1$, with $\zeta_0=1$. Since the sum of the series entering Eq. (10) changes from $8/\pi^2$ for $n=0$ to 1 for $n=\infty$, the asymptotic form of ζ_n for large n is given by just the prefactor in Eq. (10). It follows that the power series (9) converges absolutely for $|u| < \infty$, thus defining the function $\varphi(u)$, which is analytic for any finite value of u. This function equals unity at $u=0$ and attains its asymptotic form $\varphi_a(u)=\sqrt{\pi/2u}\,\exp(-1/2u)$ for $u \gtrsim 2$. Indeed, the relative difference between φ and φ_a is 6.7% for $u=1$, only 0.8% $u=2$, and becomes completely negligible for $u \gtrsim 3$.

Consequently, for $u \gtrsim 2$ one can write the scaling law

$$\tilde{\chi}_s^a(u)=(\pi/2u)^{1/2}\exp[\tfrac{1}{8}\pi^2 u-(1/2u)]\ , \tag{12}$$

which is peculiar to the strong correlation regime. It should be emphasized that, since $\tilde{\chi}_s^a/\tilde{\chi}_K=\exp(-1/2u)$, the susceptibility tends rather slowly towards its limiting Kondo value $\tilde{\chi}_K$, but the strong correlation regime is established as soon as χ_s assumes its asymptotic form (12), i.e., for $u \gtrsim 2$. We also mention that $\tilde{\chi}_c$ becomes exponentially small in the strong correlation regime, so that $\tilde{\gamma}\cong\frac{1}{2}\tilde{\chi}_s$ for $u\gtrsim 2$.

In the perturbative approach of Yoshida and Yamada[6] to the symmetric Anderson model the Hamiltonian is divided into the unperturbed part, equal to the nonmagnetic Hartree-Fock approximation to the full Hamiltonian, and the perturbation $U(n_{d\uparrow}-\frac{1}{2})(n_{d\downarrow}-\frac{1}{2})$, so that only the effect of fluctuations is treated perturbatively. The macroscopic quantities are then expanded in the power series of $u=U/\pi\Delta$, with the coefficients given in terms of the imaginary-time integrals of the determinants built from the one-particle temperature Green functions for the unperturbed Hamiltonian. As regards the susceptibilities, the Yosida and Yamada result for $T=0$ can be written as

$$\tilde{\chi}_s(u)=\sum_{n=0}^{\infty}C_n u^n\ , \tag{13}$$

$$\tilde{\chi}_c(u)=\sum_{n=0}^{\infty}(-1)^n C_n u^n\ , \tag{14}$$

where the coefficients C_n are given in terms of n-dimensional integrals. The first five coefficients have been obtained by Yamada,[7] who evaluated the appropriate integrals, while the high-order terms are too complicated to be calculated directly even by numerical methods. Since the determinantal method is not restricted to a summation of a certain class of diagrams (rather, it takes into account all the diagrams of a given order), it could be used for establishing the exact relations between different quantities of the model. Thus Yamada[7] shows that $\tilde{\gamma}^{(n)}=\frac{1}{2}[\tilde{\chi}_s^{(n)}+\tilde{\chi}_c^{(n)}]$.

In order to compare these results with those obtained by means of the Bethe-ansatz method we multiply the series expansion of $\exp(\frac{1}{8}\pi^2 u)$ and the power series (9) together and re-collect the terms of the same order to obtain $\tilde{\chi}_s$ and $\tilde{\chi}_c$ in the form of (13) and (14). Using the recursion relation (11) for ζ_n's we find that coefficients C_n are given as the solution of the set of linear equations

$$C_n=(2n-1)C_{n-1}-(\pi/2)^2 C_{n-2} \tag{15}$$

for $n\geq 2$, with $C_0=C_1=1$. It is seen at once that the first five C_n's generated by Eq. (15) coincide with Yamada's result. Assuming that the susceptibilities have unique series expansions in powers of $U/\pi\Delta$, it follows that, due to the high symmetry of the functions that enter the integrals in the theory of Yosida and Yamada, the n-dimensional integral for C_n could be reduced to a sum of lower-order terms according to Eq. (15). Thus, the complete perturbative solution could be constructed by iteration.

The solution of Eq. (15) for general n can be written as

$$C_n=[(\tfrac{1}{2}\pi)^{2n+1}/(2n+1)!!]P_n\ , \tag{16}$$

$$P_n=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\frac{(2n+1)!!}{[2(n+k)+1]!!}\left[\frac{\pi^2}{8}\right]^k\ , \tag{17}$$

and since $2/\pi=P_0\leq P_n\leq P_\infty=1$, it is easy to see that the power series (13) and (14) representing $\tilde{\chi}_s$ and $\tilde{\chi}_c$ converges absolutely for $|u| < \infty$. We are thus led to the conclusion that both $\tilde{\chi}_s$ and $\tilde{\chi}_c$ are analytic functions for any finite value of u and that the perturbation theory in terms of u is appropriate and gives exact results not only for small u, but for any finite u. Furthermore, since the magnitude of C_n decreases rapidly with increasing order [$C_n\cong(\pi/2)^{2n+1}/(2n+1)!!$ for large n], even a limited number of terms in Eqs. (13) and (14) is sufficient for an accurate description of the system, not just in the weak correlation regime but in the strong correlation regime as well. Thus, e.g., for Wilson's ratio $R(u)=\tilde{\chi}_s/\tilde{\gamma}$ at $u=2$ the finite-order approximations give $R^{(4)}=1.889$, $R^{(6)}=1.952$, and $R^{(8)}=1.961$, while the exact value at $u=2$ is $R=1.962$.

We mention here that the determinantal perturbation expansion has been used[9–11] to show that in the strong correlation regime the low-temperature behavior of the model obeys scaling laws. That is, both the transport and the thermodynamic quantities become universal functions when written in terms of the reduced variables T/Θ and

$(\mu_B h)/(k_B\Theta)$, where $k_B\Theta = \Delta/\pi\tilde{\gamma}$. The coefficients of $(T/\Theta)^n$ and $[(\mu_B H)/(k_B\Theta)]^n$ in the appropriate low-temperature and/or low-field expressions become parameter independent for $\mu \gtrsim 2$. Here, as in the case of Wilson's ratio, the finite-order perturbation theory is found to describe accurately the transition to the strong correlation regime. For example, the coefficient $\kappa_\rho = \frac{1}{3}[1+2(R-1)^2]$ of the $(T/\Theta)^2$ term of the electrical resistance, which equals 1 in the $u \to \infty$ limit, is equal to 0.950 at $u=2$, while the finite-order approximations give $\kappa_\rho^{(4)} = 0.860$, $\kappa_\rho^{(6)} = 0.938$, and $\kappa_\rho^{(8)} = 0.949$. Clearly, any finite-order approximation must break down eventually for sufficiently large u, but once the crossover region has been passed (which happens at $u \sim 1$), the scaling laws can be used to extrapolate the results to an arbitrary point in the strong correlation region.

To conclude, we have shown that the spin susceptibility, charge susceptibility, and the specific-heat coefficient for the symmetric Anderson model can be represented by power-series expansions that converge for any finite value of the expansion parameter $U/\pi\Delta$. These expansions rapidly assume their asymptotic form so that for $U/\pi\Delta \gtrsim 2$ the strong correlation behavior characterized by scaling laws is obtained. The finite-order approximation is seen to be able to reproduce the scaling laws, which lends support to the belief that one could use the perturbative approach of Yoshida and Yamada to write down the series expansions for the quantities that could not be evaluated by the Bethe-ansatz method, calculate the first several terms, and obtain the results that retain their validity both in the weak correlation and the strong correlation regimes.

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