Temperature-Dependent Susceptibility in the Anderson Model and its Universality

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A Green's function which is asymptotically exact in the Kondo regime is presented. The temperature-dependent susceptibility of the Anderson model is calculated from this Green's function and is found to be in excellent agreement at all temperatures with the results of renormalization-group theory. The formalism presented suggests a microscopic physical mechanism for the scaling and universality of the thermodynamic properties found in renormalization-group theory.

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We present a Green's function for the Anderson model[1] which satisfies the Baym condition[2] for the macroscopic conservation of momentum, energy, and number of particles and which is asymptotically exact in the limit of small mixing parameter V between the impurity d state and the host conduction band. The resultant calculated magnetic susceptibility is in excellent agreement with the results of renormalization-group theory[3] (hereinafter referred to as RGT) for all temperatures. Furthermore, our formalism suggests a microscopic physical mechanism for the scaling of the parameters of the model and, being based on Green's functions, offers a more immediate physical interpretation and perhaps a more immediate extension to other more realistic models.

Recently, the Anderson Hamiltonian has been formally diagonalized.[4] Also, recent calculations[5,6] of the thermodynamic properties of the Kondo Hamiltonian based on the Bethe *Ansatz* have given excellent agreement with RGT. However, these calculations, being numerical, do not reveal the physical mechanism responsible for the scaling. How the temperature dependence of the susceptibility comes about in the Anderson model is not known. There exists only the conjecture that a central peak at the Fermi level is somehow responsible.[7]

We calculate the Green's function by applying the functional derivative method developed[8] for the Hubbard model. Two-particle Green's functions, Γ, involved in the equation of motion for the d-electron Green's function, G, are replaced by functional derivatives $\delta G/\delta V$ with respect to arbitrary external fields, δV, which transfer d electrons to conduction-band states, k, and vice versa:

$$\Gamma(tt') = \delta G(tt')/\delta V(t) + G'(tt)G(tt').$$

If $\delta G/\delta V$ is neglected, the resulting G_0 is identical to that obtained under decoupling approximations. If $\delta G/\delta V$ is evaluated iteratively starting from $G_0(tt')$, under the assumption that the equal-time Green's function $G'(tt)$ is independent of δV, all possible diagrams in powers of V^2 can be generated.[9] On the other hand, if $G'(tt)$ is independent of δV, the original functional differential equation is reduced to an ordinary differential equation which can be solved exactly by a power-series expansion. The resultant Green's function given by

$$G_{d\sigma}^{-1} = \frac{(\omega-\omega_1)(\omega-\omega_2)}{\omega-(1-\langle N_{d\bar{\sigma}}\rangle)U} - \frac{S(\omega)[\omega-(1-\langle N_{d\bar{\sigma}}\rangle)U]^4}{(\omega-\omega_K)(\omega-\omega_P)(\omega-\omega_A)(\omega-\omega_B)}, \quad (1)$$

has three principal peaks, with the lower and upper peaks approximately at the energies ω_1 and ω_2 respectively, and a central peak associated with the energy ω_K approximately at the Fermi level. The energies ω_P, ω_A, and ω_B are associated with additional peaks to be discussed, the equal-time Green's functions $\langle N_{d\sigma}\rangle$ and $\langle N_{d\bar{\sigma}}\rangle$ are equal to the occupation numbers $n_{d\sigma}$ and $n_{d\bar{\sigma}}$, respectively, in this approximation, and

$$S(\omega) = \sum_k |V_{dk}|^2/(\omega-\epsilon_k),$$

where ϵ_k is a conduction-band energy. Although this result corresponds to the exact sum of all

possible diagrams in many-body perturbation theory, it is divergent. For example, the formulas for ω_K and ω_P involve terms of the form

$$\sum_k (V+\delta V)_{dk} \frac{\langle c_{d\bar{\sigma}}^{\dagger} c_{k\bar{\sigma}} \rangle}{[\langle N_{d\sigma}\rangle - \langle N_{d\bar{\sigma}}\rangle]} + \text{H.c.}$$

which diverge because $n_{d\bar{\sigma}} = n_{d\sigma}$.

The $G_{d\sigma}(\omega)$ obtained above is, of course, not a self-consistent solution; when G is inserted into the original equation, δV operates on equal-time Green's functions, $\langle N_{d\sigma'}\rangle$, etc., yielding new types of terms. We can, however, expand the $\langle N_{d\sigma'}\rangle$, etc., involved in $G(\omega)$ in powers of δV and determine the coefficients of the first derivatives in such a way that G is a self-consistent solution, provided second- and higher-order derivatives are neglected. This results in a renormalization of the $N_{d\sigma'}$ so that

$$\langle N_{d\sigma'}\rangle \equiv n_{d\sigma'} + \Phi_{\sigma}(d\sigma') \tag{2}$$

in the expression for $G_{d\sigma}(\omega)$.[8] The first-order corrections $\Phi_{\sigma}(d\sigma)$ and $\Phi_{\sigma}(d\bar{\sigma})$ to $n_{d\sigma}$ and $n_{d\bar{\sigma}}$ are distinct and thus eliminate the divergences discussed above, yielding a renormalized and well-behaved $G_{d\sigma}$. These corrections are of order $(V^2/DU)^{1/3}$, where D is the conduction bandwidth and U is the strength of the intra-atomic Coulomb interaction. If one were to extend the calculation one step further by evaluating second derivatives, the resultant second-order corrections would be of second order in $(V^2/DU)^{1/3}$. Hence, the first corrections are necessary in order to avoid divergences, but higher-order corrections are small in the Kondo regime. Thus, the Green's function given by (1) and (2) is asymptotically exact, satisfies all conservation laws, and within errors of order $(V^2/DU)^{2/3}$ is self-consistent.

Unfortunately, the solution of Eqs. (1) and (2) together with the associated self-consistent equations for the renormalization functions $\Phi_{\sigma}(d\sigma)$ and $\Phi_{\sigma}(d\bar{\sigma})$ and the energies ω_1, ω_2, ω_K, ω_P, ω_B, and ω_A is next to impossible by only iterative methods. However, the correct self-consistent physical solution to these equations can be found by physical insight and further formal analysis. We propose on physical grounds two essential characteristics of any correct solution and describe a self-consistent three-peaked Green's function which possesses those characteristics, gives a minimum in the free energy lower than that given by a simple two-peaked function, and gives the correct susceptibility.

The energies ω_1 and ω_2 in Eq. (1) lie approximately at the lower and upper peaks of the d-electron spectral-weight function, $A_{d\sigma}(\omega)$; ω_K, ω_P and either ω_B or ω_A lie between ω_1 and ω_2, with the other energy, say ω_A, lying either below ω_1 or above ω_2. The three energies, $\omega^{(K)}$, $\omega^{(P)}$, and $\omega^{(B)}$, which give the exact positions of those peaks in $A_{d\sigma}(\omega)$ which lie between ω_1 and ω_2 can be calculated from the zeros of $G_{d\sigma}^{-1}$. Upon defining $6\gamma = \omega_P - \omega_K$ and $3(\delta - \gamma) = \omega_K - \omega_B$, one can rewrite Eq. (1) in the dimensionless form

$$\left[\frac{\omega-\omega_K}{\delta}\right]\left[\frac{\omega-\omega_K-6\gamma}{\delta}\right]\left[\frac{\omega-\omega_K-3(\gamma-\delta)}{\delta}\right] = -i\left[\frac{\chi(\omega)}{\delta^3}\right], \tag{3}$$

where

$$-i\chi(\omega) = S(\omega)\frac{[\omega-(1-\langle N_{d\bar{\sigma}}\rangle)U]^5}{(\omega-\omega_1)(\omega-\omega_2)(\omega-\omega_A)},$$

and $S(\omega)$ is purely imaginary for the symmetric Anderson model.

In general, the imaginary parts of the roots $\omega^{(K)}$, $\omega^{(P)}$, and $\omega^{(B)}$ are of order $(V^2/DU)^{1/3}$; however, if $\chi(\omega)/\delta^3$ is sufficiently small ($\lesssim 1$), there exists some value of the ratio γ/δ for which one of the roots becomes real. We postulate on physical grounds that one of the roots, say $\omega^{(K)}$, should lie at the Fermi level, $\mathrm{Re}\{\omega^{(K)}\} = \mu$, and should be very nearly real at $T = 0$. We then find that the broad spectral peaks associated with the other two roots are unobservable. Furthermore, the reality of $\omega^{(K)}$ fixes the value of γ/δ as a function only of $\chi(\omega)/\delta^3$. Self-consistency then uniquely specifies the value of $\chi(\omega)/\delta^3$ and hence that of γ/δ, so that both are independent of V, D, and U. Thus, Eq. (3) is completely scaled. This scaling gives rise to the universality observed in RGT. Because the form of Eq. (3) is unchanged by including terms of higher order in $(V^2/DU)^{1/3}$, corrections to this universality must be of order $k_B T/U$ or smaller.

The energy shift at $T = 0$, $\Delta K \equiv \mathrm{Re}\{\omega^{(K)}\} - \omega_K$, can be expressed as a rapidly convergent power series in $\chi(\omega)/2\delta^3$,

$$\Delta K(\delta) = -\delta \sum_{n=2}^{\infty} C_n(\gamma/\delta)\,(\chi/2\delta^3)^n, \tag{4}$$

where the C_n's depend only on the fixed value of γ/δ, with $C_2 \simeq 0.19$. The actual self-consistent value of γ/δ depends upon temperature, introducing a temperature-dependent width, $\Delta_K \equiv \alpha(T) k_B T$, in the central peak. Assuming $k_B T \ll U, D$ and postulating that the central peak must be pinned at the Fermi level, one finds that the increase with temperature of the free energy of the system

is given by $\Delta E(T) = \Delta(T) - \Delta(0)$ with

$$\Delta E(T) = -\int \frac{d\omega}{2\pi} \frac{2\Delta_K}{(\omega-\mu)^2+\Delta_K^2} \Delta K(\delta(\omega,T)) f(\omega), \tag{5}$$

where $\delta(\omega, T)$ is a slowly varying function of ω with

$$\delta(\mu, T) = \delta_T = \delta_0 + \delta_1 k_B T + \delta_2 \ln\{[1+\alpha^2(T)]^{1/2} k_B T/D\}. \tag{6}$$

Here, the factor $[1+\alpha^2(T)]^{1/2}$ arises from the Lorentzian form of the central peak, and the ln term arises from the Kondo integral in such two-particle collision terms as

$$\zeta_0(\omega) = \iiint \prod_{i=1}^{3} \frac{d\omega_i}{2\pi} \sum_k \frac{|V_{dk}|^2}{\omega_2 - \epsilon_k} \frac{[\epsilon_k - (1-\langle N_{d\bar\sigma}\rangle)U]^4}{(\epsilon_k-\omega_K)(\epsilon_k-\omega_P)(\epsilon_k-\omega_A)(\epsilon_k-\omega_B)} \times \frac{A_{d\sigma}(\omega_1)A_{d\bar\sigma}(\omega_2)A_{d\bar\sigma}(\omega_3)}{\omega-\omega_1+\omega_2-\omega_3} F(\omega_1)F(\omega_3)[1-f(\epsilon_k)],$$

which occur in the equations for the renormalization functions $\Phi_\sigma(d\sigma;\omega)$. Substituting Eqs. (4) and (6) into Eq. (5) and integrating, one finds

$$\Delta E(T) \simeq C_2 |\chi/2\delta_T^3|^2 \left\{\delta_0 + \delta_1' k_B T + \left[\delta_2 - \frac{10\alpha(T)}{3\pi\gamma/\delta} k_B T\right] \ln([1+\alpha^2(T)]^{1/2}(T/T_L))\right\}, \tag{7}$$

where

$$\delta_1' = \delta_1 - [10\delta\alpha(T)/3\pi\gamma]\ln[k_B T_L/D]$$

and T_L is the temperature at which the universal curve of $k_B T\chi(T)$ vs $\ln(k_B T/D)$ has an inflection point (the transition temperature between the strong-coupling and localized-moment regimes). We have found that the pinning of $\omega^{(K)}$ at the Fermi level, independent of temperature, is self-consistent. Physically, this pinning is associated with the fact that the central peak arises from two-particle collision terms.

Mathematically, it arises from the necessity that the renormalization functions $\Phi_\sigma(d\sigma')$ be large compared to V^2/DU in order to obtain self-consistency. This condition, which is associated with the rough inverse proportionality of the energies ω_K, ω_P, ω_B, and ω_A to the $\Phi_\sigma(d\sigma')$, can be satisfied only if the Kondo integrals in such collision terms as $\zeta_0(\mu)$ are large, hence, only if $\omega^{(K)}$ is at or very near the Fermi level.

Because the central peak is narrow and Lorentzian, it should have the properties of a quasiparticle peak; in particular, $\Delta E(T)$ should be very nearly proportional to $k_B T$. In the low-temperature limit, $T \ll T_L$, this yields the results $\alpha(T) = T_L/T$, $\Delta_K = k_B T_L$ and $\delta_2 = 10\, k_B T_L/3\pi(\gamma/\delta)$, while in the high-temperature limit, $T \gg T_L$ (but $T \ll D, U$), it gives $\alpha(T) = \ln 10/\ln(T/T_L)$. That the last term on the right-hand side of Eq. (7) must be proportional to T implies that

$$[\alpha(T) - T_L/T]\ln\{(T/T_L)[1+\alpha^2(T)]^{1/2}\} = \ln 10. \tag{8}$$

The condition $\Delta E(T) \propto k_B T$ has been found to be self-consistent.

We have proven rigorously that contributions to the susceptibility from the lower and upper peaks cancel exactly, and that the susceptibility is completely determined by the central peak according to the formula

$$\frac{\chi(T)}{(g\mu_B)^2} = \int_{-\infty} \frac{d\omega}{2\pi} \frac{2\Delta_K}{(\omega-\mu)^2+\Delta_K^2} \left[-\frac{\partial f(\omega)}{\partial\omega}\right] \tag{9}$$

with $\Delta_K \equiv \alpha(T)\, k_B T$ determined from Eq. (8). Equations (6), (8), and (9) thus determine T_L and $\chi(T/T_L)$, and hence T_K/T_L, where T_K, the Kondo temperature, is defined by the equation,

$$k_B T_K \chi(T_K) = 0.07(g\mu_B)^2,$$

as in RGT. Because of our assumption that $T \ll U, D$ in Eqs. (5) and (9), we obtain a universal curve for $\chi(T/T_L)$ and hence a universal value $T_K/T_L = 0.65$. Our results for $k_B T\chi(T)$ as a function of T/T_L are in excellent quantitative agreement down to $T/T_L \sim 0.1$ with the results of RGT as is shown in Fig. 1. However, we find $k_B T_L \chi(T)/(g\mu_B)^2$ to approach the constant value π^{-1} in the low-temperature limit, as compared with the value 0.15 found numerically by RGT. Our results for T_L (or T_K) are obtained with much less precision, but they are in agreement with the results of RGT within their quoted uncertainty. For $U = 10^{-3}D$ and the two values 0.064 and 0.8 for $\rho J_{\rm eff} \equiv 8\rho|V|^2/U$, RGT obtained $k_B T_K \simeq 3.7\times10^{-12}D$ and $k_B T_K \simeq 0.6\times10^{-4}D$; we obtained $k_B T_K \simeq 2.5\times10^{-12}D$ and $k_B T_K \simeq 0.6\times10^{-4}D$, respectively.

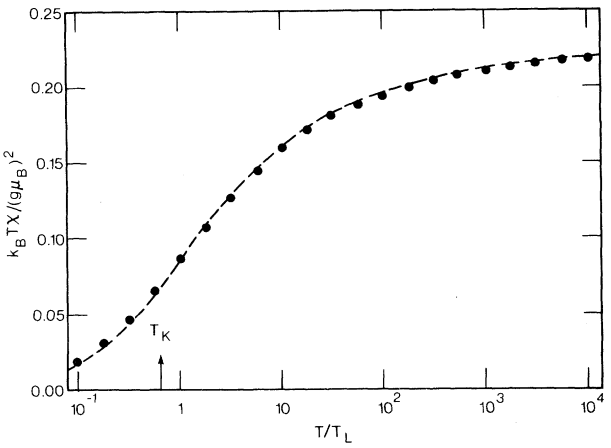

FIG. 1. The universal function $k_B T\chi(T)/(g\mu_B)^2$ as a function of T/T_L, where T_L is the temperature at which the function has an inflection point. The dots show the values found in this paper for the Anderson model; dashed curve shows the results of RGT for the Kondo model. The arrow indicates the value of the Kondo temperature as defined by RGT.

In summary, physical reasoning has led us to postulate two basic properties for any physical Green's function for the Anderson model: (1) the existence of a sharp central peak in $A_{d\sigma}(\omega)$ at the Fermi level and (2) a quasiparticle-like dependence on temperature of the free energy, $\Delta(T)$, associated with the central peak. A Green's function having these properties has been constructed self-consistently, with use of the condition of minimization of the free energy as an aid in its calculation. The Green's function found is asymptotically exact in the Kondo regime and yields a temperature-dependent susceptibility in excellent quantitative agreement with the results of RGT. The Green's function constructed gives rise to a spectral-weight function, $A_{d\sigma}(\omega)$, which has only three observable peaks, the very narrow central peak at the Fermi level and the usual two peaks approximately at ϵ_k and $\epsilon_k + U$. The width of the central peak varies from $1.6\, k_B T_K$ in the low-temperature limit up to $k_B T \ln 10/\ln(T/1.6T_K)$ at high temperatures. Both the pinning of the central peak and its width can be understood physically and mathematically in terms of the collision processes which give rise to it.

A complete mathematical derivation of the results given here and a more precise specification of the Green's function, $G_{d\sigma}$, will be given elsewhere.

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