Application of tridiagonalization to the many-body problem. II. Finite T

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In a previous paper of the same title, we obtained the ground-state energy of a magnetic (Wolff-model) impurity in a nonmagnetic metal. In the present Brief Report, we calculate the impurity's contribution to the density of states and heat capacity of the metal at low temperatures. Here, the Lanczös reduction ("tridiagonalization") converges less rapidly, so that our results are of qualitative merit only. Nevertheless, we confirm the validity of perturbation theory in the weak-coupling regime, and find, at strong coupling, that the interaction introduces an extra fraction $2/N$ of states at the Fermi level.

I. INTRODUCTION

We continue the study of a magnetic impurity in the Wolff-model approximation,[1] initiated in a previous paper,[2] henceforth denoted I. The magnetic character of the impurity is the result of a two-body Coulomb repulsion of strength U between any two electrons on the impurity. This interaction is ignored in the rest of the solid and is the only feature distinguishing the impurity from the hosts. The contribution to the ground-state energy from this perturbation was found to be $O(U^2)$ for $U \ll 1$ in units of the bandwidth. At large U, a smooth crossover to a linear dependence on U, the strong-coupling regime, characterized the breakdown of perturbation theory.

In the present Brief Report, we investigate the low-temperature heat capacity of the metal + impurity. This retains its form, characteristic of a metal, $c=\gamma T$ at low temperature T ($T \ll T_k$ or $T \ll T_F$). The coefficient γ changes, however, depending on U. We calculate $c(U,T)-c(0,T) \equiv \delta c(U,T)$, a quantity which is independent of the size of the system and is characteristic of the impurity. At low temperature, it too takes the form $\delta c = \delta\gamma T$ linear in the temperature, and it is the coefficient that we seek.

Our calculation scheme in this many-body problem is the same as in I, viz., tridiagonalization. We carry out the scheme only to the level of a 3×3 matrix. The method has its practical limitations; carrying it out to higher matrices or to higher powers of T is too cumbersome to do manually. Further improvements will therefore await the development of computer algorithms for calculating the type of information in Tables I and II, the entries in which we are still doing by hand calculations.

II. METHOD

We refer to I for the statement of the method and discussion of the chosen Hamiltonian. The novelty here is in our choice of the initial state about which to tridiagonalize, replacing the Fermi sea $|F\rangle$ in I by a state with one quasiparticle excitation

$$\phi_0 = c^\dagger_{k\uparrow}|F\rangle \text{ or } c^\dagger_{k\downarrow}|F\rangle, \text{ energy } \epsilon_k \geq 0 , \tag{1a}$$

for $k > k_F$, or

$$\phi_0 = c_{k\uparrow}|F\rangle \text{ or } c_{k\downarrow}|F\rangle, \ \epsilon_k \leq 0 , \tag{1b}$$

for $k < k_F$. Repeated applications of H to any given ϕ_0 then generates a tridiagonal matrix.[2] The eigenstates of each such matrix (for a given k) constitute an orthonormal set, each member of which is orthogonal to the eigenstates for a different k. We are only interested in the lowest energy state in each set, and denote it E_k.

We illustrate with (1a). The relevant algebraic elements are given in the accompanying Table I. The calculated numbers are the result of integrations, assuming a flat density of states (DOS) as in I.

Table II lists the first few tridiagonal matrix elements, obtained from Table I. It remains to obtain the lowest eigenvalue, which represents the energetic cost E_k to promote a quasiparticle at $k > k_F$. We illustrate the procedure with a 2×2 matrix, for which it is easy to follow the explicit calculations. Noting that the Fermi level is at $\epsilon_k = 0$, we diagonalize

$$M = \begin{pmatrix} \epsilon_k & -\frac{1}{4}U \\ -\frac{1}{4}U & 1+\epsilon_k - 4\epsilon_k/N \end{pmatrix} \tag{2}$$

and obtain

$$E_k = \epsilon_k\left[1-\frac{2}{N}[1-(1+\tfrac{1}{4}U^2)^{-1/2}]\right] . \tag{3}$$

By symmetry, the same result is obtained for a hole just below the Fermi level. We conclude that the DOS at the Fermi level $\epsilon = 0$ is effectively changed from an initial value ρ_0 to a new value ρ:

$$\rho = \rho_0\left[1-\frac{2}{N}[1-(1+\tfrac{1}{4}U^2)^{-1/2}]\right]^{-1} . \tag{4}$$

In general, one can cast ρ in the form

$$\rho = \rho_0\left[1+\frac{1}{N}g(U)+O(1/N^2)\right] . \tag{5}$$

In the 2×2 approximation we denote g by $g_2(U)$, and after comparing (4) and (5) obtain

$$g_2(U) = 2-2(1+\tfrac{1}{4}U^2)^{-1/2} , \tag{6}$$

observing that in the strong-coupling limit ($U \gg 2$) $g_2 \to 2$; i.e., it appears as if a fraction of $2/N$ of states is added to the available total DOS near the Fermi surface. Without invoking any physical interpretation, we observe that $g_3(U)$ also tends to 2 in the strong-coupling limit, and

TABLE I. Relevant matrix elements ($\epsilon_{ij} \equiv \epsilon_i - \epsilon_j$). Algebraic quantities required in the construction of the tridiagonal matrix, and their evaluation in the case of a constant DOS $\rho_0(\epsilon) = 1$, $-\frac{1}{2} < \epsilon < +\frac{1}{2}$.

$$\Gamma_1 = \frac{1}{N^2}\sum_{qq'}\sum_{pp'}\langle F|c_{k\uparrow}c^\dagger_{q\uparrow}c_{q'\uparrow}c^\dagger_{p\uparrow}c_{p'\uparrow}c^\dagger_{k\uparrow}|F\rangle\epsilon_{q'q}\epsilon^2_{pp'} = \frac{3}{64} - \frac{\epsilon_k}{4N} - \frac{\epsilon_k^3}{N}$$

$$\Gamma_2 = \frac{1}{N^2}\sum_{qq'}\sum_{pp'}\langle F|c_{k\uparrow}c^\dagger_{q\uparrow}c_{q'\uparrow}c^\dagger_{p\uparrow}c_{p'\uparrow}c^\dagger_{k\uparrow}|F\rangle\epsilon_{q'q}\epsilon_{pp'} = \frac{7}{96} - \frac{\epsilon_k}{2N}$$

$$\Gamma_3 = \frac{1}{N}\sum_{qq'}\langle F|n_{0\downarrow}c^\dagger_{q\downarrow}c_{q'\downarrow}|F\rangle\epsilon_{qq'} = \frac{1}{8}, \quad n_{0\downarrow} = \frac{1}{N}\sum_{kk'}c^\dagger_{k\downarrow}c_{k'\downarrow}$$

$$\Gamma_4 = \frac{1}{N}\sum_{qq'}\langle F|n_{0\downarrow}c^\dagger_{q\downarrow}c^\dagger_{q'\downarrow}|F\rangle\epsilon^2_{qq'} = \frac{7}{96}$$

$$\Gamma_5 = \frac{1}{N}\sum_{qq'}\langle F|c_{k\uparrow}c^\dagger_{q\uparrow}c_{q'\uparrow}n_{0\uparrow}c^\dagger_{k\uparrow}|F\rangle\epsilon_{qq'} = \frac{1}{8} - \frac{\epsilon_k}{N}$$

$$\Gamma_6 = \langle F|c_{k\uparrow}n_{0\uparrow}c^\dagger_{k\uparrow}|F\rangle = \frac{1}{2} + \frac{1}{N}$$

$$\Gamma_7 = \frac{1}{N^2}\sum_{qq'}\sum_{pp'}\langle F|c^\dagger_{q\downarrow}c_{q'\downarrow}c^\dagger_{p\downarrow}c_{p'\downarrow}|F\rangle\epsilon_{q'q}\epsilon_{pp'} = \frac{7}{96}$$

$$\Gamma_8 = \frac{1}{N^2}\sum_{qq'}\sum_{pp'}\langle F|c^\dagger_{q\downarrow}c_{q'\downarrow}c^\dagger_{p\downarrow}c_{p'\downarrow}|F\rangle\epsilon_{q'q}\epsilon^2_{pp'} = \frac{3}{64}$$

$$\Gamma_9 = \frac{1}{N}\sum_{qq'}\langle F|c_{k\uparrow}c^\dagger_{q\uparrow}c_{q'\uparrow}n_{0\uparrow}c^\dagger_{k\uparrow}|F\rangle\epsilon^2_{qq'} = \frac{7}{96} - \frac{\epsilon_k}{2N}$$

$$\langle F|c_{k\uparrow}\Omega H_0\Omega c^\dagger_{k\uparrow}|F\rangle = 4(\Gamma_3+\Gamma_5) = 1 + \epsilon_k - \frac{4\epsilon_k}{N}$$

$$[\Omega \equiv (2n_{0\uparrow}-1)(2n_{0\downarrow}-1)] \ .$$

$$\langle F|c_{k\uparrow}\Omega H_0^2\Omega c^\dagger_{k\uparrow}|F\rangle = (4\Gamma_2+4\Gamma_7+32\Gamma_3\Gamma_5) + 8(\Gamma_3+\Gamma_5)\epsilon_k + \epsilon_k^2 = 1.08333 + 2\epsilon_k - \frac{2\epsilon_k}{N}(3+4\epsilon_k)$$

$$\begin{aligned}\langle F|c_{k\uparrow}\Omega H_0^3\Omega c^\dagger_{k\uparrow}|F\rangle &= (4\Gamma_1+32\Gamma_2\Gamma_3+16\Gamma_4\Gamma_5+16\Gamma_3\Gamma_9+32\Gamma_5\Gamma_7+4\Gamma_8)\\ &\quad+(8\Gamma_2+4\Gamma_4+8\Gamma_7+4\Gamma_9+96\Gamma_3\Gamma_5)\epsilon_k+12(\Gamma_3+\Gamma_5)\epsilon_k^2+\epsilon_k^3\\ &= 1.25+3.25\epsilon_k+3\epsilon_k^2+\epsilon_k^3-7.5\frac{\epsilon_k}{N}-18\frac{\epsilon_k^2}{N}-16\frac{\epsilon_k^3}{N}\end{aligned}$$

TABLE II. Tridiagonal matrix. First seven nontrivial matrix elements of the tridiagonal matrix.

$$m_{00} = \epsilon_k$$

$$m_{01} = \frac{-U}{4} = m_{10}$$

$$m_{11} = \langle F|c_{k\uparrow}\Omega H_0\Omega c^\dagger_{k\uparrow}|F\rangle = 4(\Gamma_3+\Gamma_5)+\epsilon_k = 1+\epsilon_k-4\frac{\epsilon_k}{N}$$

$$\begin{aligned}m_{12} &= -[\langle F|c_{k\uparrow}\Omega(H_0-m_{11})^2\Omega c^\dagger_{k\uparrow}|F\rangle]^{1/2} = -[4\Gamma_2+4\Gamma_7-16\Gamma_3^2-16\Gamma_5^2]^{1/2}\\ &= -\left(\frac{1}{12}+2\frac{\epsilon_k}{N}\right)^{1/2} = m_{21}\end{aligned}$$

$$\begin{aligned}m_{22} &= \frac{1}{m_{12}^2}\langle F|c_{k\uparrow}\Omega(H_0^3-2H_0^2m_{11}+m_{11}^2H_0)\Omega c^\dagger_{k\uparrow}|F\rangle\\ &= [4\Gamma_2+4\Gamma_7-16\Gamma_3^2-16\Gamma_5^2]^{-1}[(4\Gamma_1+4\Gamma_8+32\Gamma_2\Gamma_3+16\Gamma_4\Gamma_5+16\Gamma_3\Gamma_9+16\Gamma_5\Gamma_7)\\ &\quad+(8\Gamma_2+4\Gamma_4+8\Gamma_7+4\Gamma_9+96\Gamma_3\Gamma_5)\epsilon_k+12(\Gamma_3+\Gamma_5)\epsilon_k^2+\epsilon_k^3]\\ &= 1+\epsilon_k+14\frac{\epsilon_k}{N}+24\frac{\epsilon_k^2}{N}-48\frac{\epsilon_k^3}{N}\end{aligned}$$

conjecture that this strong-coupling limit is, in fact, exact. At the opposite limit, in weak coupling, $g(U) \propto U^2$, a feature in agreement with perturbation theory.[3]

III. HEAT CAPACITY

The heat capacity of an electron gas at low temperature is proportional to the temperature T and to the DOS at the Fermi level. Thus, we find the excess heat capacity associated with the impurity to be

$$\delta c = \frac{1}{N} g(U) \gamma_0 T \ , \tag{7}$$

where $\gamma_0 T$ is the heat capacity of the metal at $U=0$ (i.e., with a host atom replacing the single impurity). As γ_0 is $O(N)$, N being the total number of atoms $>> 1$, the product $(1/N)\gamma_0$ is $O(1)$. The qualitative features of δc can be obtained from $g_2(U)$ in (6).

Proceeding to the solution of the cubic eigenvalue equation for the 3×3 tridiagonal matrix, we obtain $g_3(U)$ numerically, as plotted in Fig. 1. Because the variational basis is larger, the $n=3$ solution must be more accurate than $n=2$. In fact, the *qualitative* features of $g_3(U)$ in weak- and strong-coupling regimes are seen in Fig. 1 to be the same as for $g_2(U)$, although quantitatively they still differ by a substantial amount. One would wish to be able to calculate $g_n(U)$, $n=4, 5, \ldots$ until, as in I, convergence has been established. Unfortunately, the requisite algebra is still beyond our ability to perform conveniently at the present time, and $g_3(U)$ merely represents our best estimate of the $g(U)$. It establishes the general shape: concave (parabolic) at small U, and convex for $U > 1$, becoming asymptotic to 2 at $U >> 1$.

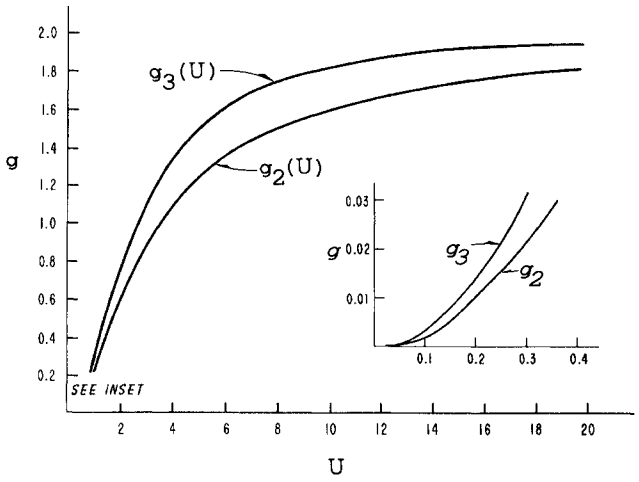

FIG. 1. $g_n(U)$ for $n=2$ and $n=3$. $g_n(U)/N$ is the fractional increase in the electronic density of states at the Fermi level, for N electrons on N atoms; U is the strength of the two-body repulsion on the magnetic impurity atom, and n is the order of approximation in the tridiagonal scheme. The specific heat associated with the defect is $\delta c = [g(U)/N]\gamma_0 T$.

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[1]P. A. Wolff, Phys. Rev. 124, 1030 (1961).
[2]J. D. Mancini and D. C. Mattis, Phys. Rev. B 28, 6061 (1983).
[3]D. Mattis, Ann. Phys. (N.Y.) 89, 45 (1975), Eq. (2.30). The use of Tomonaga operators in this paper is equivalent to summing all diagrams in perturbation theory.