Ground state of the Kondo model

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(Received 29 January 1985)

The single-impurity Kondo problem is investigated with the use of the nonperturbative Lanczos (tridiagonalization) method. We are able to obtain an explicit expression for the ground-state energy in terms of the Kondo coupling constant J. The method places no restrictions on the range of J.

I. INTRODUCTION

The problem of a single spin-$\frac{1}{2}$ magnetic impurity coupled to the conduction band of a nonmagnetic host metal, the so-called Kondo problem, has been the subject of a great deal of work by many authors. Of particular note is the work of Wilson[1] and Andrei, Furuya, and Lowenstein.[2] Wilson utilized renormalization-group techniques to make calculations on the susceptibility and specific heat of this model, but not the ground-state energy. Andrei *et al.*, using the Bethe ansatz, obtained expressions for the ground-state energy and excitation spectrum, as well as for the thermodynamic functions. However, their expression for the ground-state energy involves a rather complex dependence on the cutoff. This dependence makes comparisons of this expression with other works impractical.[3] Our purpose here is to obtain an expression for the ground-state energy which is neither cutoff dependent nor perturbative in nature.

In this Brief Report we wish to report on the continuation of work initiated by us on the application of the nonperturbative Lanczos method (tridiagonalization) to the many-body problem.[4,5] In particular, we shall investigate the ground state of Kondo's Hamiltonian[6]

$$H = H_0 + H_{\text{int}} \ . \tag{1}$$

TABLE I. List of relevant matrix elements.

$$\langle\phi_0|H|\phi_0\rangle = 0$$

$$\langle\phi_0|H^2|\phi_0\rangle = \frac{3J^2}{8}$$

$$\langle\phi_0|H^3|\phi_0\rangle = \frac{3J^2}{16} + \frac{3J^3}{8}$$

$$\langle\phi_0|H^4|\phi_0\rangle = \frac{7J^2}{64} + \frac{3J^3}{8} + \frac{21J^4}{32}$$

$$\langle\phi_0|H^5|\phi_0\rangle = \frac{9J^2}{128} + \frac{41J^3}{128} + \frac{63J^4}{64} + \frac{15J^5}{16}$$

$$m_{00} = \langle\phi_0|H|\phi_0\rangle = 0$$

$$m_{10} = m_{01} = \frac{-\langle\phi_0|H^2|\phi_0\rangle}{\langle\phi_0|H^2|\phi_0\rangle^{1/2}} = -J\sqrt{3/8}$$

$$m_{11} = \frac{\langle\phi_0|H^3|\phi_0\rangle}{\langle\phi_0|H^2|\phi_0\rangle} = \frac{1}{2} + J$$

$$m_{12} = m_{21} = -[\langle\phi_0|H^4|\phi_0\rangle - m_{11}\langle\phi_0|H^3|\phi_0\rangle + m_{10}^2\langle\phi_0|H^2|\phi_0\rangle] \times [\langle\phi_0|H^2|\phi_0\rangle]^{-1/2} = -\left[\frac{1}{24} + \frac{5J^2}{4}\right]^{1/2}$$

$$m_{22} = m_{12}^{-2}[\langle\phi_0|H^5|\phi_0\rangle - 2m_{11}\langle\phi_0|H^4|\phi_0\rangle + m_{11}^2\langle\phi_0|H^3|\phi_0\rangle] \times [\langle\phi_0|H^2|\phi_0\rangle]^{-1} + \frac{2m_{10}}{m_{12}^2}[\langle\phi_0|H^3|\phi_0\rangle - m_{11}\langle\phi_0|H^2|\phi_0\rangle] \times [\langle\phi_0|H^2|\phi_0\rangle]^{-1/2} = \frac{1 + 20J + 18J^2}{2 + 60J^2}$$

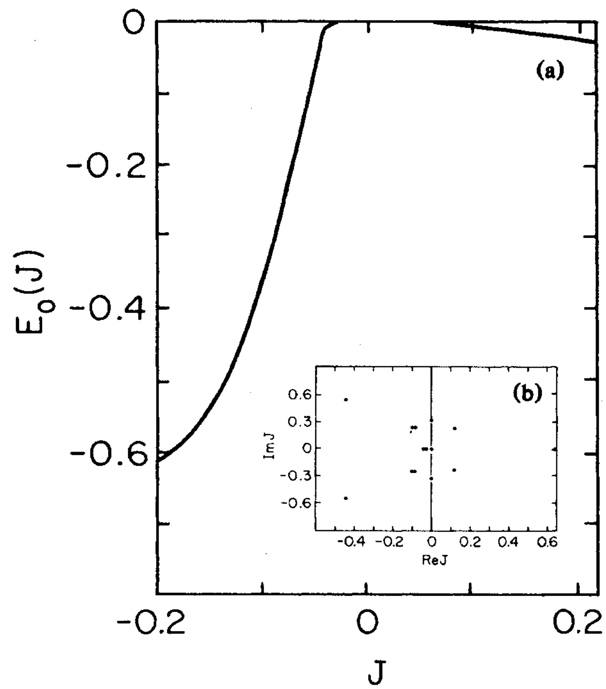

FIG. 1. (a) The ground-state energy E_0 is plotted as a function of the coupling J. The calculation was carried out to third order in the tridiagonalization scheme. Higher-order calculations would yield more information on the exact shape of the curve. (b) Inset. We have examined E_0 as a function of *complex J*. Calculation on the 3×3 submatrix yields 18 branch points, which are shown here.

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H_0 is diagonal:

$$H_0=\sum_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma}\epsilon_k \ , \tag{2}$$

and the interaction Hamiltonian is given by

$$H_{\rm int}=-J(n_{0\uparrow}-n_{o\downarrow})S_z - Jc^\dagger_{o\uparrow}c_{o\downarrow}S_- - Jc^\dagger_{o\downarrow}c_{o\uparrow}S_+ \ , \tag{3}$$

where

$$c_{o\sigma}=\frac{1}{(N)^{1/2}}\sum_k c_{k\sigma}\ , \quad n_{o\sigma}=\frac{1}{N}\sum_{kk'} c^\dagger_{k\sigma}c_{k'\sigma} \ .$$

The subscript "o" denotes the fact that we have chosen the spin-$\frac{1}{2}$ impurity to be localized about the origin. By convention, we have chosen the parameter J to be a constant (i.e., not a function of k and k').

In the spirit of (4) and (5), we define the ground state of the system

$$|\phi_0\rangle = |F\rangle\alpha \ , \tag{4}$$

where $|F\rangle$ denotes the filled Fermi sea and α denotes the "up" spinor $\binom{1}{0}$.

Once again our purpose is to generate the tridiagonal Hermitian matrix $\tilde{M}$ whose elements m_{ij} are given by

$$H|\phi_i\rangle = m_{i,i-1}|\phi_{i-1}\rangle + M_{i,i}|\phi_i\rangle + m_{i,i+1}|\phi_{i+1}\rangle \ . \tag{5}$$

Diagonalization of any submatrix of $\tilde{M}$ yields a variational upper bound on the ground-state energy E_0.

II. RESULTS

Table I lists the relevant matrix elements obtained. The numerical values are obtained by explicit evaluation of the integrals using a flat density of states. The calculation was terminated at the 3×3 level. This is due to the level of complexity of the expressions which were obtained manually. However, the results are still of qualitative merit, as can be seen by Fig. 1(a). Higher-order calculations of $\tilde{M}$, and subsequent diagonalization, would yield more information on the exact shape of the curve.

The tridiagonalization scheme also allows us to investigate the ground-state energy as a function of the *complex* coupling J. The calculation for the 2×2 submatrix of $\tilde{M}$ is straightforward, and yields branch points at $J=\frac{1}{3}(1\pm i/2)$. The branch points for $\tilde{M}$ of dimension 3×3 are given in Fig. 1(b).

This study allows us to focus on the failure of various weak-coupling schemes which are seen to be limited to the range dictated by the radius of convergence of the power series expansions. The method employed in this work has no such limitation, and in principle any range of coupling may be investigated.

ACKNOWLEDGMENT

The authors gratefully acknowledge the support of the National Science Foundation, Grant No. DMR 81-06223.

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