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# Strongly correlated electron ground-state energy approximations for Anderson-like models

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We report preliminary results of convergence properties for nonperturbative resolvent approximations to Anderson-like models of magnetic ions in metals. Our study is initially focused on the spin-$\frac{1}{2}$ Anderson model for magnetic impurities, but the methods studied can include multiplet and crystal-field effects which are needed for more accurate descriptions of real systems. We will compare the nonperturbative Lanczos method (tridiagonalization) and similar truncation schemes to exact ground-state energies for the impurity model and assess the efficacy of these nonperturbative approaches to understanding the Anderson lattice, heavy fermions, and other strongly interacting electronic systems.

Mancini and Mattis[1] examined a variational method for evaluating the ground state of the Wolf Hamiltonian by analytically evaluating the matrix elements of the Hamiltonian for an orthonomal basis set of states generated from the tridiagonalization of the Hamiltonian matrix given an initial state. The initial state that was used in the case of the Wolf Hamiltonian was simply the filled Fermi sea. The remaining states in the orthonormal sequence were sums of all particle excitations and more complicated composite many-particle states. This selection of states is in contrast to more traditional variational treatments, such as that by Varma and Yafet,[2] in the context of the Anderson magnetic impurity model where the orthonormal variational states were chosen to be the individual particle-hole excitations. With such individual excitation states the resulting Hamiltonian matrix is essentially infinite in dimension, and the ground-state eigenvalue must be estimated by solving a transcendental equation. The primary difficulty with this traditional method is that it is difficult to construct a sequence of approximations that systematically improves on the ground-state energies obtained by using only the simplest particle-hole excitations. The matrix truncation scheme of Mancini and Mattis combines the different particle-hole excitations into composite states and thus results in a sequence of finite dimensional matrices. This sequence is guaranteed to converge as the size of the matrix increases though the rate of convergence may be slow. The nature of the sequence of states is expected to be the factor that most strongly effects the rate of convergence.

The most surprising result of the Mattis and Mancini study was the quick convergence of the ground-state eigenvalues and the corresponding estimate that this sequence gave for the ground state of the system.

A further benefit arising from the analytic tridiagonalization is that explicit expressions for the matrix elements were obtained whose analytic structure as functions of model parameters could be studied. Since these matrix truncations schemes are nonperturbative the examination of these explicit expressions enabled discussion of the range of validity of perturbations expansions. The major disadvantage is the complexity of the matrix elements as the size of the truncation dimension is increased. A large amount of algebraic manipulation is required whenever a somewhat complex initial variational state is chosen and the size of the truncation is to exceed $5 \times 5$.

An alternative to the analytic tridiagonalization which has the promise of yielding tractable higher-order truncations is to relax the requirement that the matrix be tridiagonal, but to continue to explore the use of composite variational states in the matrix expansion. This approach would begin with some state such as the filled Fermi sea and generate an orthonormal sequence of composite states by constructing the matrix of the Hamiltonian and choosing states by a criterion that different states need represent different physical processes and be as simple as possible. Such an approach gives rise to a very tractable sequence of states and has the possibility of large truncations for a modest effort. If the convergence is found to be relatively fast, this may be a way of getting numerical estimates of ground-state energies of systems of interest such as the lattice Anderson model and other systems of strongly correlated electrons. This nontridiagonal approach does not allow an anallytic study of Hamiltonian parameters, but these questions may be studied numerically.

One of the motivations of this preliminary study is to reexamine the surprisingly fast convergence of Mattis and Mancini for another Hamiltonian with exact eigenvalues. The results reported here arise from application to the inpurity spin-$\frac{1}{2}$ Anderson model and will be extended to the lattice model elsewhere.

For this paper we compare a $3 \times 3$ tridiagonalization and an $18 \times 18$ nontridiagonal truncation with each other and with various exact results for the Anderson impurity model. The Anderson $H$ is written as follows:

$$H = \sum_{ks} \epsilon_{ks} n_{ks} + \sum_{s} \epsilon_{fs} N_s + U N_+ N_- + \sum_{ks} \frac{V}{\sqrt{N}} (f_s^\dagger c_{ks} + c_{ks}^\dagger f_s) , \quad (1)$$

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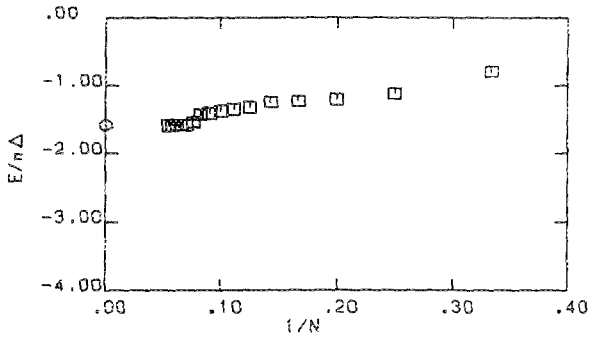


FIG. 1. The lowest eigenvalue $E/\pi\Delta$ of each truncation $N$ is plotted against $1/N$ for $N=3,18$. The squares show the nontridiagonalized approximanst. The circle on the $y$ axis shows the variational energy of Gunnarson and Schönhammer.

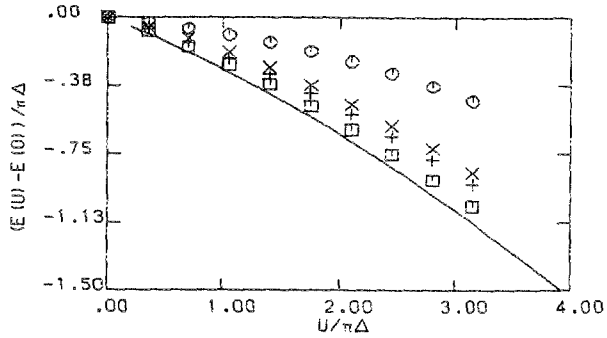


FIG. 2. The deviation of the lowest eigenvalue from its $U=0$ value is plotted against $U$ for the symmetric Anderson model. The solid line represents a Bethe anzatz calculation (Ref.3) and circles represent a $3\times3$ truncation, $\times$'s a $8\times8$, crosses a $12\times12$, and squares an $18\times18$ truncation. Both axis are normalized to $\pi\Delta$.

where $n_{ks}=c_{ks}^{\dagger}c_{ks}$ and $N_s=f_s^{\dagger}f_s$, and where $c_{ks}^{\dagger}$ and $f_s^{\dagger}$ are creation operators for the conduction-electron and localized $f$-electron orbitals, respectively. The conduction-electron energies are $\epsilon_{ks}$, $\epsilon_{fs}$ represent the atomic orbital energies of the $f$ electrons, $U$ is the Coulomb matrix element between the localized orbitals, and $V$ is the hybridization matrix element between the conduction electrons and the localized orbitals. We write the ket $|F\rangle$ to represent the filled Fermi sea multiplied by the no-electron state of the localized orbitals. This product state is the beginning state for both of the sequences that will be studied here and for even numbers of conduction electrons lies in the same subspace that we expect for the singlet ground state of this Hamiltonian. For the purposes of this study we use a constant density of conduction electron states with a bandwidth $w$ and assume that the hybridization $V$ is independent of the wave vector $k$. Operating on $|F\rangle$ with $H$ yields the following first row for the $H$ matrix:

$$H|F\rangle=E_0|F\rangle+\frac{V}{\sqrt{N}}\sum_{ks}f_s^{\dagger}c_{ks}|F\rangle\,, \tag{2}$$

where $E_0$ is the energy of the half-filled conduction band. In the truncation approximations studied here we take the second term in Eq.(2) as our next orthogonal vector and proceed to construct the next rows of the $H$ matrix by acting on it with $H$.

The Varma–Yafet and Gunnarson–Schönhammer approach chooses each $k$-dependent state $f_s^{\dagger}c_{ks}|F\rangle$ as an independent vector state and finds as an approximate ground-state eigenvalue equation for the case when $\epsilon_{fs}$ is below the conduction-band bottom. The variational ground state is of the form

$$|\psi\rangle\propto|F\rangle+\frac{1}{\sqrt{N}}\sum_{k}\frac{V}{(\epsilon_f-\epsilon_{ks}-E)}f_s^{\dagger}c_{ks}|F\rangle\,. \tag{3}$$

A semiquantitative connection between this variational state and our truncation sequence may be made by noting that for large $\epsilon_{fs}$ the denominator can be expanded in a power series in $\epsilon_{ks}/\epsilon_{fs}$. In the orthonormal sequence of states generated in this method the terms of this expansion in moments of the conduction band will be found. Thus the orthonormal sequence of vectors will recover parts of Eq.(3) as well as more complicated many-electron states such as conduction-electron–hole states, two-electron–two-hole states, etc. It is this connection between the usual variational states and the inclusion of more complicated basis states that gives us hope for this truncation method.

The analytic tridiagonalization method and the nontridiagonal methods agree when the appropriate truncations are compared. The nontridiagonal matrices were carried out to $18\times18$ truncations including both spin states with an external magnetic field and those results will be compared with the Bethe anzatz results below. This level of truncation was not difficult to derive since the matrix is quite sparse.

The first question which must be examined is the rate of convergence. Figure 1 shows the dependence of the lowest eigenvalue as function of the reciprocal of the matrix dimension. The small squares represent the nontridiagonal approximants and the circle on the vertical axis represents the variational solution of Varma and Yafet or Gunnarson and Schönhammer for this large value of $U/\pi\Delta\approx3.5$. As can be seen, the sequence is tending to converge as expected, though the steps in the sequence as the truncation dimension increases is somewhat surprising. The steps seem to be decreasing as $N$ increases. The agreement is quite good.

To make contact with the Bethe anzatz we compare the $U$ dependence of the ground-state energy with the Kawakami and Okiji[3] calculation of the Wiegmann solution for the spin-$\frac{1}{2}$ model. It is important to realize that as $U$ is varied $\epsilon_{fs}=-0.5U$, preserving the symmetric Anderson model. The comparison of the deviation of the normalized ground-state energy from its $U=0$ value as a function of $U/\pi\Delta$ is shown in Fig. 2. Both axes of this figure are normalized to $\pi\Delta$ where $\Delta=\pi V^2/w$. The solid line is the Kawakami and Okiji solution and the symbols show the result of various truncations. The circles represent the simplest $3\times3$ or $2\times2$ (tridiagonalized) truncation. The $\times$'s represent the $8\times8$, the crosses represent the $12\times12$, and the squares represent the $18\times18$ truncation.

In summary, matrix truncations of the Hamiltonian using composite states that contain sums over the conduction-electron excitations seem to represent a convergent sequence with moderately fast convergence. It would seem that somewhat larger truncations than those considered here could yield ground-state estimates that might be useful for the study of more complex model Hamiltonians. This promising preliminary study is not enough to decide whether the con-

vergence rate for this type of basis state is fast enough to merit its widespread use in the study of heavy-fermion and other strongly correlated systems. However, it appears worthwhile to pursue these questions in detail elsewhere.

[1]J. D. Mancini and D. C. Mattis, Phys. Rev. **31**, 7440 (1985); **29**, 6988 (1984); **28**, 6061 (1983).
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