ANL/MSD/PP-72490

MANY ELECTRON VARIATIONAL GROUND STATE OF THE TWO DIMENSIONAL ANDERSON LATTICE*

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FEBRUARY 1991

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Patent Cleared by
Patent Department ANL
DATE 4/14/91 BY David R. Hamrin
Technical Information Services, ANL

Submitted to Phys. Lett. A.

*Work Supported by the U.S. Department of Energy, BES-Materials Sciences, under
Contract W-31-109-ENG-38.

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Many Electron Variational Ground State of the Two Dimensional Anderson Lattice

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Abstract

A variational upper bound of the ground state energy of two dimensional finite Anderson lattices is determined as a function of lattice size (up to 16×16). Two different sets of many-electron basis vectors are used to determine the ground state for all values of the coulomb integral U . This variational scheme has been successfully tested for one dimensional models and should give good estimates in two dimensions.

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In this brief work we wish to consider the ground state energy of the two dimensional Anderson lattice[1]. The method which we employ here is the Lanczos variational scheme[2]. This method involves initially choosing a trial wavefunction $|\psi_0\rangle$ which in general may depend on variational parameters. Then the variational estimate for the ground state energy is given by:

$$E_0 = \frac{\langle \psi_0 | H | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} \quad (1)$$

provided that $|\psi_0\rangle$ is not orthogonal to the true ground state. We can generate a subspace that may contain the true ground state by the operation[3]

$$|\psi_n\rangle = H^n |\psi_0\rangle \quad (2)$$

If we let M_k denote the subspace spanned by $|\psi_n\rangle$ with $k \geq n \geq 0$, then the ground state energy is given by

$$E_{gs} = \lim_{k \rightarrow \infty} E_k \quad (3)$$

where

$$E_k = \min \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle} \quad (4)$$

and $|\phi\rangle \in M_k$. Thus by constructing a larger basis the ground state energy may be better approximated.

We consider the symmetric periodic Anderson lattice model:

$$H = \sum_{ks} \epsilon_{ks} c_{ks}^\dagger c_{ks} + \sum_{ls_1} E_l f_{ls_1}^\dagger f_{ls_1} + U \sum_l f_{l\uparrow}^\dagger f_{l\uparrow} f_{l\downarrow}^\dagger f_{l\downarrow} + \frac{V}{\sqrt{N}} \sum_{kls} (e^{i\vec{k} \cdot \vec{R}_l} f_{ls_1}^\dagger c_{ks_1} + \text{H.c.}) \quad (5)$$

where the $c^\dagger$ (c) and $f^\dagger$ (f) represent creation (annihilation) operators for the conduction d-orbital and localized f-orbital electrons respectively. The parameter U represents the Coulomb energy of the localized orbitals and V is the hybridization energy. In Eq.(5),

$$\epsilon_{ks} = -2t (\cos(k_x) + \cos(k_y)) . \quad (6)$$

We choose our initial trial many-particle wavefunction to be the filled Fermi-sea of conduction electrons and N singly occupied f-orbitals where N denotes the number of sites. We then construct a basis according to Eq.(2). Care is taken to orthonormalize the vectors generated according to a Gram-Schmidt procedure. The basis we have chosen is a 13 dimensional subspace, and is identical to the basis chosen to study the symmetric one-dimensional periodic Anderson ring[4]. The 13-state basis includes single particle-hole excitations, two particle-hole excitations, and RKKY-type interactions.

Since we have kept a fixed 13x13 many-particle basis regardless of the size of a lattice, the calculations can be carried out for moderately large sizes with fairly small amount of computing time. The results of the ground state energies per site as functions of U for 4x4, 8x8 and 16x16 lattices are shown in Fig.1, in which we have chosen $t=0.5$ and $V=0.375$, consistent with the calculations for one-dimension[4-5]. It is seen that in the vanishing U limit, the larger the lattice size becomes, the higher the variational ground state energy is. We attribute this to the fact that at small U , the true ground state is spanned in a much larger space of states than the subspace of the 13-state-basis used here. And the larger the lattice, the more the basis states there are that overlap

the ground state wavefunction. For small U the actual band structure near the Fermi energy should dominate in the system, while the vectors which appear in our calculation represent the band energies by averages over the whole band. For large U (symmetric Anderson model) the ground state will be dominated by singly occupied f states as are the 13×13 basis in this calculation. For this reason we expect the variational calculation should work well in the large U limit as in one-dimension case[4]. Similar to the property of one-dimensional Anderson calculation[6], our ground state energy results here show little size effect in the relevant large U parameter range.

While we do not expect our results to be valid at the mixed-valence regime (small U), it is useful to apply another simple approximation in this vanishing U limit, so that an upper bound is given for the ground state energy by combining the results of the two calculations. If we use the exact many-particle wavefunction for $U=0$ as our variational state, then the approximated ground state energy is obtained by finding the expectation value of the Hamiltonian in this state[4]:

$$E_0(U) = \sum_{ks} \lambda_{ks}(-) + \frac{U}{N} \left[\sum_k \frac{V^2 + (\lambda_{ks}(-) - \epsilon_{ks})^2}{(\lambda_{ks}(+) - \lambda_{ks}(-))^2} \right]^2 \quad (7)$$

where

$$\lambda_{ks}(\pm) = \frac{1}{2} (\epsilon_{ks} + E_{fs}) \pm \frac{1}{2} \sqrt{(\epsilon_{ks} - E_{fs})^2 + 4V^2} \quad (8)$$

are the exact energies of the hybridized bands for $U=0$. Thus at $U=0$, eq.(7) yields exact ground state energy of the model. The results of this simple estimate are shown along with our variational calculations for 4×4 , 8×8 and 16×16 lattices in Fig.2.

Since results show the similarities between one-dimensional and two-dimensional systems, it should be interesting to compare the ground state energy per site of a two-dimensional lattice with

that of a one-dimensional ring with the same number of sites. In Fig.2, we also compare a 4x4 square lattice ground state energy with that of a 16-site ring[4], and an 8x8 square with a 64-site ring[4] respectively for our variational calculation in 13 basis states. All of the parameters are the same as those used in Fig.1. Despite the similar shapes of the plots, a two-dimensional lattice always has a lower ground state energy than a one-dimensional lattice with the same number of sites. Qualitatively, this is because each atom in a square lattice has 4 nearest-neighbor sites while it has only 2 nearest-neighbors in a ring. Therefore, for a square lattice, each basis state couples with more other states, generating more non-zero off-diagonal elements in the Hamiltonian matrix, which accounts for a lower ground state energy.

Because a small truncated basis has been used, as well as the fact that those vectors representing excitations close to the Fermi energy have been left out, we do not expect to get a good approximation of any ground state property which has a strong dependence on the wavefunction. Some of these properties have been studied with exact diagonalization and Monte Carlo method by Callaway et.al.[7-8]. However, using a Lanczos variational scheme within a finite basis, we have obtained reasonable results of ground state energy of up to 16x16 square lattice with small amount of effort, and the approximation can be further improved by choosing a larger basis of states.

Acknowledgement

This work is supported by the U.S. Department of Energy, BES-Materials Sciences, under Contract #W-31-109-ENG-38. One of us (JDM) gratefully acknowledges the support of a grant from the Research Corporation and from a Fordham University Faculty Fellowship.

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Figure Captions

Fig. 1: Ground state energy as a function of U for different lattice sizes: 4x4 (solid line), 8x8 (dash line) and 16x16 (dot dash line). All results are for $t = 0.5$ and $V = 0.375$.

Fig. 2: Ground state energy as a function of U for 4x4, 8x8 and 16x16 lattices. The solid line is the result of our variational calculations based on 13x13 matrices. The dashed line is the plot of Eq.(7) which approximates the small U ground state. The two lines give an upper bound to the true ground state energy. In (a) and (b), the variational results for one dimensional lattice with the same number of sites are also plotted (dot-dashed line) for comparison. Parameters are the same as in Fig.1.

Fig. 1

Fig. 2a

Fig. 2b

(c) 16x16

Fig. 2c