Many-electron variational calculation for the one-dimensional Anderson lattice

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We present a variational method for studying the ground-state properties of the one-dimensional Anderson model with periodic boundary conditions. Our results are compared with exact Monte Carlo results and show excellent agreement in the large-U limit. We argue that poor results in the vanishing-U range are due to the truncated basis chosen, as well as the fact that all fluctuations are treated equally.

I. INTRODUCTION

Recently there has been a great deal of interest in the ground-state properties of a lattice of localized moments as a description of mixed-valence systems.[1] The interesting physics of such systems arises from the interaction of the localized f orbitals (with energy close to the Fermi energy) with the conduction d bands and by the f-orbital intrasite Coulomb energy. At high temperature they tend to have isolated moments. A model appropriate to describe such systems is the periodic Anderson model (PAM). Theoretical work on this model has included perturbation expansions in the Coulomb energy U,[2] various Green's-function approaches,[3] functional-integration methods,[4] real-space renormalization,[5] and direct diagonalization of finite clusters.[6] A wide variety of variational schemes has also been applied to this model.[7] These include a number of Gutzwiller-type approaches[8] whereby an initial trial function is chosen to project out the two-particle states on the localized f orbitals. Such an approach represents a mean-field theory and thus no information regarding spin correlations of neighboring localized orbitals may be extracted. Another important work, relevant to the present study, is that of Blankenbecler *et al.*[9] who utilized a stochastic Monte Carlo technique to study the ground-state properties of the one-dimensional PAM. Comparisons with this work, which we take to represent the true ground state, shall be made throughout.

This work represents a continuation of an earlier preliminary study[10] on the Anderson model in which the localized f orbitals were found to be antiferromagnetically correlated in the ground state via a Ruderman-Kittel-Kasuya-Yosida (RKKY) type of interaction. In this paper a variational ground-state energy as well as magnetic correlation functions and hybridization matrix elements are evaluated. The method utilizes a finite matrix truncation scheme whereby a limited subspace of the full Hamiltonian is generated.[11] The power of the method lies in the fact that for modest computation times one may study very large systems with extensions to higher dimensions being straightforward. A drawback of the technique is that excitations near the Fermi energy are approximated as average band energies thus obscuring any information on low-lying energies leading to the Fermi-liquid behavior of intermediate valence systems. We study here the ground-state properties of the one-dimensional PAM for an 8-site, 16-site, 32-site, and 64-site lattice. Comparisons are made with a stochastic Monte Carlo calculation performed on a 16-site chain. Our results are in excellent agreement with those of the Monte Carlo calculations in the Kondo lattice regime (Coulomb energy U large). However, in the mixed valence parameter range our results are rather disappointing. This we argue is a consequence of choosing a finite basis whereby important vectors containing the hybridization matrix elements as well as those which represent excitations close to the Fermi energy have been left out. We shall reserve further discussion on this matter until the final section.

The paper is organized as follows. In Sec. II we discuss the method and the set of vectors chosen to span the subspace of the PAM Hamiltonian. We also introduce a diagrammatic representation of these vectors which facilitates the choosing of a linearly independent set of vectors as well as rendering the orthogonalization (via a Gram-Schmidt orthogonalization process) of this set more manageable. In Sec. III we give our results and comparisons with other methods are made. Discussion and conclusion are given in Sec. IV.

II. FORMALISM

The Hamiltonian for the nondegenerate one-dimensional periodic Anderson model has the form

$$H=\sum_{k,s}\varepsilon_{ks}c_{ks}^{\dagger}c_{ks}+\sum_{l,s_l}E_l f_{ls_l}^{\dagger}f_{ls_l}+U\sum_{l}f_{l\uparrow}^{\dagger}f_{l\uparrow}f_{l\downarrow}^{\dagger}f_{l\downarrow}$$
$$+\frac{V}{\sqrt{N}}\sum_{k,l,s}(e^{i\mathbf{k}\cdot\mathbf{R}_l}f_{ls_l}^{\dagger}c_{ks_l}+\text{H.c.})\,, \tag{1}$$

where $c^{\dagger}$ (c) and $f^{\dagger}$ (f) are the creation (annihilation) operators for the conduction d-orbital and localized f-orbital electrons, respectively. Here U is the on-site Coulomb energy of the localized f electrons. V represents the hybridization of the two bands, taken to be k independent, and

$$\varepsilon_{k,s} = -2t\cos(k) , \tag{2}$$

where t is the hopping energy and $-\pi < k \leq \pi$. In this work we shall consider particle-hole symmetry with $E_l = -U/2$, and for numerical calculations we use a linear dispersion for the conduction electrons $-1 \leq \varepsilon_k \leq 1$. The calculation is variational and we choose our initial trial wave function to consist of a filled Fermi sea of conduction electrons together with a set of singly occupied localized orbitals.

We denote the filled Fermi sea of conduction electrons with the symbol $\cup$ and the set of singly occupied localized orbitals by a horizontal line $\overset{1}{\text{—}\bullet\text{—}}$, where l denotes a particular site. Hence the initial trial wave function is represented by

$$|\phi_1\rangle = |\Omega\rangle \equiv \; | \cup \text{—} \rangle \tag{3}$$

with the normalization $|\phi_1|^2 = 1$.

A truncated basis consisting of various particle-hole excitations may be constructed by repeated operations of Eq. (1) on $|\Omega\rangle$. The set of states generated may be represented diagrammatically, with rules for their construction not given here. Repeated operations of the Hamiltonian[12] yield a set of nineteen vectors. After checking for linear independence and performing a Gram-Schmidt orthogonalization, the basis was reduced to a set of thirteen independent vectors. Each of these vectors represents a different physical excitation of the ground state. We shall be interested in obtaining the lowest eigenvalue of the 13×13 Hamiltonian matrix within this basis. This matrix is both small and sparse allowing the calculations to be performed on a desk-top computer using standard matrix routines. It is hoped that such a small amount of computational effort will yield qualitatively useful information on the ground state.

To illustrate the method, we note that explicit operation of the Hamiltonian on the initial vector $|\phi_1\rangle$ yields the following two new vectors. Each vector represents linear combinations of all distinct single particle-hole excitations,

$$\begin{aligned} |\phi_2\rangle &= \frac{1}{\sqrt{N}} \sum_{k<k_F} \sum_{l} e^{ikR_l} f^{\dagger}_{l\bar{s}_l} c_{k\bar{s}_l} |\Omega\rangle , \\ |\phi_3\rangle &= \frac{1}{\sqrt{N}} \sum_{k>k_F} \sum_{l} e^{-ikR_l} c^{\dagger}_{ks_l} f_{ls_l} |\Omega\rangle . \end{aligned} \tag{4}$$

The vector $|\phi_2\rangle$ represents the physical event whereby a conduction electron with momentum $k < k_F$ and spin $\bar{S}_l \equiv -S_l$ hybridize to a localized f orbital labeled by l with an already existing spin S_l. Vector $|\phi_3\rangle$ represents the hopping of a localized electron from site l with spin S_l to the conduction band with momentum $k > k_F$. We note that just as in Oguchi's work[8] we have that while the number of f electrons is not fixed, the total electron number is conserved. He uses this condition to determine his variational parameters. The remaining vectors are given below.

We have

$$|\phi_4\rangle = \frac{1}{\sqrt{N}} \sum_{k>k_F} \sum_{l} e^{-ikR_l} (\varepsilon_{ks_l} - E_{ls_l}) c^{\dagger}_{ks_l} f_{ls_l} |\Omega\rangle ,$$

$$|\phi_5\rangle = \frac{1}{N} \sum_{k>k_F} \sum_{l\neq l'} e^{ik(R_{l'}-R_l)} \delta_{s_l\bar{s}_{l'}} f^{\dagger}_{l's_l} c_{ks_l} c^{\dagger}_{ks_l} f_{ls_l} |\Omega\rangle ,$$

$$|\phi_6\rangle = \frac{1}{N} \sum_{\substack{k>k_F \\ k'<k_F}} \sum_{l} e^{i(k'-k)R_l} f^{\dagger}_{l\bar{s}_l} c_{k's_l} c^{\dagger}_{ks_l} f_{ls_l} |\Omega\rangle ,$$

$$|\phi_7\rangle = \frac{1}{N} \sum_{\substack{k>k_F \\ k'<k_F}} \sum_{l\neq l'} e^{i(k'R_{l'}-kR_l)} f^{\dagger}_{l'\bar{s}_{l'}} c_{k'\bar{s}_{l'}} c^{\dagger}_{ks_l} f_{ls_l} |\Omega\rangle ,$$

$$|\phi_8\rangle = \frac{1}{N} \sum_{k>k_F} \sum_{l\neq l'} e^{-ik(R_{l'}+R_l)} \delta_{s_l\bar{s}_{l'}} c^{\dagger}_{ks_l} f_{l's_l} c^{\dagger}_{ks_l} f_{ls_l} |\Omega\rangle ,$$

$$|\phi_9\rangle = \frac{1}{N} \sum_{\substack{k>k_F \\ k'>k_F}} \sum_{l\neq l'} e^{-i(k'R_{l'}+kR_l)} c^{\dagger}_{k's_l} f_{l's_{l'}} c^{\dagger}_{ks_l} f_{ls_l} |\Omega\rangle ,$$

$$|\phi_{10}\rangle = \frac{1}{\sqrt{N}} \sum_{k<k_F} \sum_{l} e^{ikR_l} (E_{l\bar{s}_l} - \varepsilon_{k\bar{s}_l}) f^{\dagger}_{l\bar{s}_l} c_{k\bar{s}_l} |\Omega\rangle ,$$

$$|\phi_{11}\rangle = \frac{1}{N} \sum_{\substack{k<k_F \\ k'<k_F}} \sum_{l\neq l'} e^{i(k'R_{l'}+kR_l)} f^{\dagger}_{l'\bar{s}_{l'}} c_{k'\bar{s}_{l'}} f^{\dagger}_{l\bar{s}_l} c_{k\bar{s}_l} |\Omega\rangle ,$$

$$|\phi_{12}\rangle = \frac{1}{N} \sum_{k<k_F} \sum_{l\neq l'} e^{ik(R_{l'}+R_l)} \delta_{s_l\bar{s}_{l'}} f^{\dagger}_{l'\bar{s}_{l'}} c_{k\bar{s}_{l'}} f^{\dagger}_{l\bar{s}_l} c_{k\bar{s}_l} |\Omega\rangle ,$$

$$|\phi_{13}\rangle = \frac{1}{N} \sum_{\substack{k>k_F \\ k'<k_F}} \sum_{l} e^{i(k'-k)R_l} f^{\dagger}_{ls_l} c_{k's_l} c^{\dagger}_{ks_l} f_{ls_l} |\Omega\rangle ,$$

in which k_F is the momentum at the Fermi surface, and δ the Kronecker delta. The collection of the diagrammatic representations of these 13 many-electron state basis vectors is shown in Fig. 1.

The ground-state energy for the truncated basis of thirteen vectors is obtained by finding the lowest eigenvalue of the Hamiltonian matrix $H_{ij} = \langle \phi_i | H | \phi_j \rangle$. These matrix elements are given in the Appendix.

III. RESULTS

In this section we wish to compare our results with those of the exact Monte Carlo calculation of Blankenbecler *et al.*,[9] and also with the strong-coupling limit. The values of parameters used are the same as those in Ref. 9: $t = 0.5$ and $V = 0.375$. In the strong-coupling regime, $U \gg \delta$, where the band gap

$$\delta = \sqrt{(1+4V^2)} - 1 \tag{5}$$

and the ground-state energy is given by

$$E_g(U) = -\tfrac{1}{2}U + \frac{2}{N}\sum_k \varepsilon_k f(\varepsilon_k) - \frac{2V^2}{N}\sum_k \frac{1-f(\varepsilon_k)}{\varepsilon_k + \frac{U}{2}} \tag{6}$$

with $f(\varepsilon_k)$ the zero temperature Fermi function.

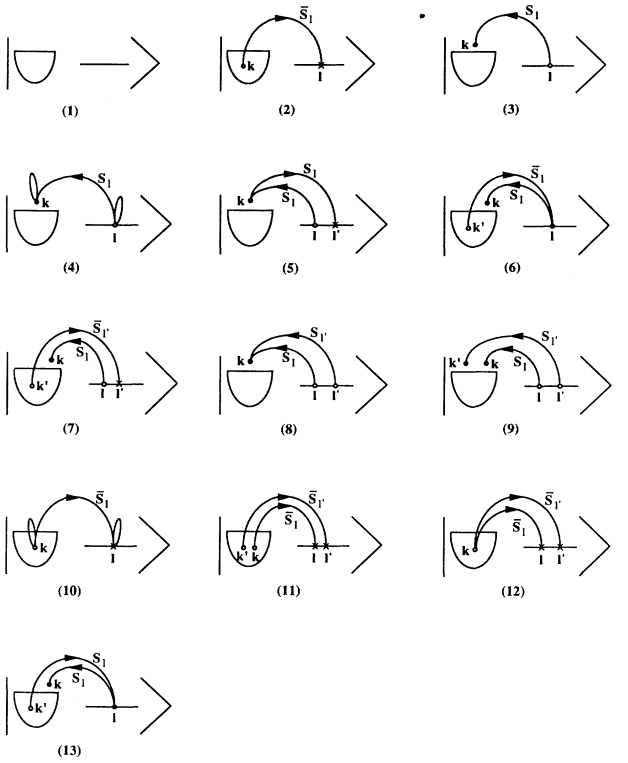

FIG. 1. Diagrammatic representation of the thirteen truncated basis states, where up to second order in particle-hole excitations with spin flips have been included. The bubbles appearing in (4) and (10) constitute correction in self-energies. Diagrams (6) and (13) are vectors which include explicitly the RKKY-type interaction.

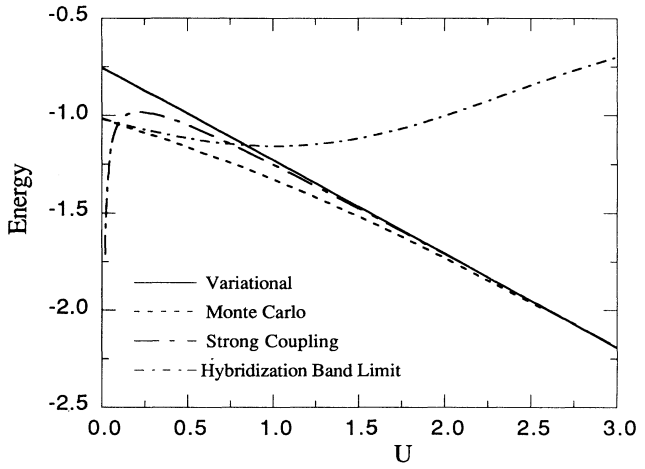

FIG. 2. Ground-state energy per site of the 16-site lattice comparing with the Monte Carlo calculation and strong-coupling approximation results. The dot-dashed line represents the small-U approximation result [Eq. (10)]. Parameters used are $t=0.5$ and $V=0.375$.

Figure 2 is a plot of the variational ground-state energy $E_0(U)$ for the sixteen-site lattice. For the large-U limit the variational ground-state energy converges quite nicely to the Monte Carlo results of Ref. 9 and for $U \geq 1.8$ are as good or better than the strong-coupling theory.

The success of this basis in the large-U limit for this symmetric Anderson model is due to the fact that particle-hole excitations with a filled f orbital and "average" conduction-band hole dominate the variational subspace. The energies of these states have the form $(-0.5U+\langle\varepsilon\rangle)$ where $\langle\varepsilon\rangle$ is an average of hole energies over the band. The Coulomb interactions between f orbitals are also treated exactly in this basis.

This variational basis does not do well for small U where the actual band structure would begin to dominate. This sequence of vectors represents the band energies by certain averages over the whole band. This characterizes the bands by a sequence of averages closely related to the cumulants of statistics. To recover the detailed band structure itself would require large numbers of these vectors. To illustrate this it is useful to examine the simplest complementary variational basis set: one which treats the hybridized bands exactly and treats the f-f Coulomb interaction in mean field only. For this sequence of many-particle states we define hybridized single-particle operators $\gamma_k^\dagger(\pm)$ to diagonalize the $U=0$ Hamiltonian. The one-electron operators are defined as

$$\gamma_{ks}^\dagger(\pm)=\frac{Vc_{ks}^\dagger+[\lambda_{ks}(\pm)-\varepsilon_{ks}]f_{ks}^\dagger}{\sqrt{V^2+[\lambda_{ks}(\pm)-\varepsilon_{ks}]^2}}\ , \tag{7}$$

where

$$\lambda_{ks}(\pm)=\tfrac{1}{2}(\varepsilon_{ks}+E_{ls})\pm\tfrac{1}{2}\sqrt{(\varepsilon_{ks}-E_{ls})^2+4V^2} \tag{8}$$

are the exact energies of the hybridized bands for $U=0$. The initial variational ground state for this sequence of states is a filled Fermi sea of $\gamma_{ks}^\dagger(-)$:

$$|G\rangle=\prod_{k,s}\gamma_{ks}^\dagger(-)|0\rangle\ . \tag{9}$$

The dot-dashed line in Fig. 2 that agrees with the Monte Carlo results at $U=0$ represents the expectation value of $\langle G|H|G\rangle$:

$$E_0(U)=\sum_{k,s}\lambda_{ks}(-)+\frac{U}{N}\left[\sum_k\frac{V^2+[\lambda_{ks}(-)-\varepsilon_{ks}]^2}{[\lambda_{ks}(+)-\lambda_{ks}(-)]^2}\right]^2\ . \tag{10}$$

In Fig. 3 we plot the ground state energy for 8-, 32-, and 64-site lattices. In the large-U limit where diagonal terms of the Hamiltonian matrix elements dominate and thus where our truncation does well, the energy per site decreases slightly as the size of the lattice increases. As the lattice size is allowed to increase, the number of states present in the true ground state also increases. Thus it is seen then that in the mixed-valence regime (small U), for larger and larger lattices our finite basis becomes a poorer approximation.

Further investigation of Fig. 3 shows that there is another effect to be considered. As U becomes very large the doubly occupied sites which appear in the true ground state will have a vanishingly small amplitude.

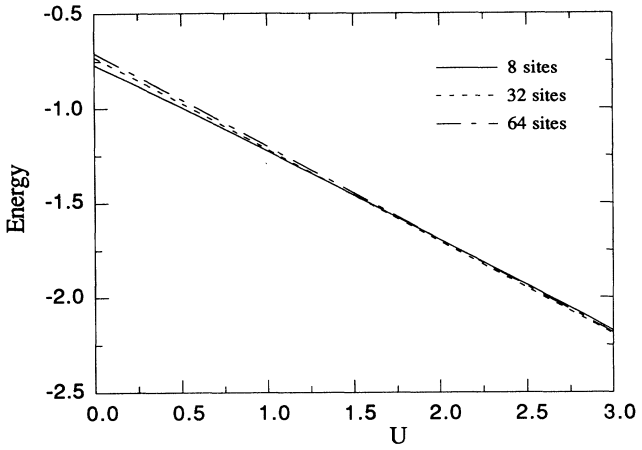

FIG. 3. Ground-state energy per site of 8-, 32-, and 64-site lattices for the same parameters as those used in Fig. 2. Note in the mixed-valence regime (small U), the energy of smaller cluster is lower than that of the larger ones in the present approximation.

Thus if one were to ignore such states then the effective number of states in the true ground state would be diminished, tending to improve any finite basis truncation scheme. Thus one needs to investigate the full range of parameter space for a given Hamiltonian before drawing conclusions on size effects and also on the limitations involved in finite-basis methods.

The square of the f-orbital single-site magnetization $\langle m_z^f(l)^2\rangle = 1-2\langle n_{f\uparrow} n_{f\downarrow}\rangle$ is shown in Fig. 4 for a 16-site lattice. Use of the Feynman-Hellmann relation enables one to write this function in terms of a derivative of the ground-state energy,

$$\langle [m_z^f(l)]^2\rangle = -2\frac{\partial E_g}{\partial U} . \tag{11}$$

We see that once again our results compare favorably in

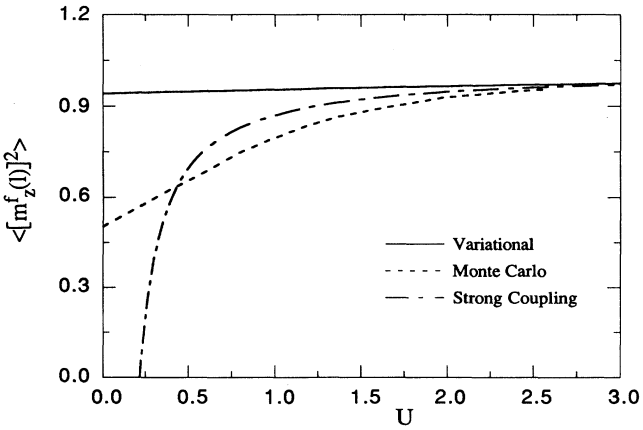

FIG. 4. The square of the f-orbital single-site magnetization vs U for a 16-site lattice.

the large-U limit with the Monte Carlo results of Ref. 9, but fail completely in the mixed-valence regime because of the poor approximation to the ground-state wave function.

It is interesting to investigate the interplay between the Coulomb energy U and the effective hybridization V. As pointed out by Blankenbecler *et al.*,[9] a useful measure of this is given by the ratio of $(f_{ls}^\dagger c_{ls} + c_{ls}^\dagger f_{ls})$ in the interacting ground state to the $U=0$ ground state. Results of Ref. 9 demonstrate that the effect of U is to decrease the hybridization. Our calculation of this quantity using the 13×13 basis yields very poor results as expected. We would expect better agreement if more states which couple to the Coulomb energy were added to the basis.

IV. CONCLUSION

By using a Lanczos-type of variational method, we have studied the ground-state properties of a one-dimensional periodic Anderson model. With a fairly small amount of computing time, we achieved excellent agreement with the exact Monte Carlo result on the ground-state-energy calculation of a 16-site lattice in the large-U limit. With a fixed number of basis states, this method allows us to carry out the calculation for much larger size lattices easily. But for this same reason (limited number of basis states), our results for properties strongly depending on the wave function of the ground state are poor. Also, we included particular linear combinations of many-electron states representing a particular phasing (constant phase) of particle-hole excitations both close to the Fermi energy and far away from it in energy. The importance of the other linear combinations of excited states in the variational ground state particularly for small hybridization is emphasized by the poor showing of these "fixed phase" excited states that are mixed into the system. We expect that they can be improved by increasing the size of the truncated matrix, thus taking account of more basis states. Since the formalism introduced here does not depend on the dimensionality explicitly, it can be easily applied to multidimensional models. The calculation of the ground-state energy of the two-dimensional Anderson lattice model using this variational scheme is presented elsewhere.[13]

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APPENDIX

With un-normalized basis vectors $|\phi_1\rangle$ through $|\phi_{13}\rangle$ defined in Sec. II, the nonzero elements of the upper half of the Hamiltonian matrix are

$$H_{11}=E_0 ,$$

$$H_{12}=H_{13}=\frac{N}{2}V,\quad H_{22}=\frac{N}{2}(E_0+U-\bar{\lambda}) ,$$

$$H_{25}=\beta^2 V,\quad H_{26}=\frac{N}{4}V,\quad H_{27}=\frac{N^2}{4}V,\quad H_{2,10}=\alpha_<^2 ,$$

$$H_{2,11}=e_<^2 V,\quad H_{2,12}=\Delta^2 V,\quad H_{2,13}=\gamma^2 V ,$$

$$H_{33}=\frac{N}{2}(E_0+\lambda),\quad H_{34}=\alpha_>^2,\quad H_{35}=\beta^2 V ,$$

$$H_{36}=\frac{N}{4}V,\quad H_{37}=\frac{N^2}{4}V,\quad H_{38}=\Delta^2 V,\quad H_{39}=e_>^2 V ,$$

$$H_{3,13}=\gamma^2 V,\quad H_{44}=(E_0+\lambda)\alpha_>^2 ,$$

$$H_{55}=(E_0+U)\beta^2,\quad H_{66}=\frac{N}{4}(E_0+\mu) ,$$

$$H_{77}=\frac{N^2}{4}(E_0+U+\mu),\quad H_{88}=(E_0+2\lambda)\Delta^2 ,$$

$$H_{99}=(E_0+2\lambda)e_>^2,\quad H_{10,10}=(E_0+U-\bar{\lambda})\alpha_<^2 ,$$

$$H_{11,11}=(E_0+2U-2\bar{\lambda})e_<^2,\quad H_{12,12}=(E_0+2U-2\bar{\lambda})\Delta^2 ,$$

$$H_{13,13}=(E_0+\mu)\gamma^2 .$$

The normalization factors are

$$|\phi_1|^2=1,\quad |\phi_2|^2=|\phi_3|^2=\frac{N}{2},\quad |\phi_4|^2=\alpha_>^2 ,$$

$$|\phi_5|^2=\beta^2,\quad |\phi_6|^2=\frac{N}{4},\quad |\phi_7|^2=\frac{N^2}{4} ,$$

$$|\phi_8|^2=|\phi_{12}|^2=\Delta^2,\quad |\phi_9|^2=e_>^2,\quad |\phi_{10}|^2=\alpha_<^2 ,$$

$$|\phi_{11}|^2=e_<^2,\quad |\phi_{13}|^2=\gamma^2 .$$

The variables used above are defined as

$$\lambda=\frac{1}{N^2}\sum_{k>k_F}\sum_{l}(2\varepsilon_{ks_l}-E_{ls_l}) ,$$

$$\bar{\lambda}=\frac{1}{N^2}\sum_{k<k_F}\sum_{l}(2\varepsilon_{k\bar{s}_l}-E_{l\bar{s}_l}) ,$$

$$\alpha_>^2=\frac{1}{N}\sum_{k>k_F}\sum_{l}(\varepsilon_{ks_l}^2-\varepsilon_>^2) ,$$

$$\alpha_<^2=\frac{1}{N}\sum_{k<k_F}\sum_{l}(\varepsilon_{ks_l}^2-\varepsilon_<^2) ,$$

$$\varepsilon_>=\frac{2}{N^2}\sum_{k>k_F}\sum_{l}\varepsilon_{ks_l} ,$$

$$\varepsilon_<=\frac{2}{N^2}\sum_{k<k_F}\sum_{l}\varepsilon_{ks_l} ,$$

$$e_>^2=(N-1)\left[\frac{N}{2}-1\right]-\frac{2}{N^2}\sum_{\substack{k>k_F\\ k'>k_F}}\sum_{\substack{l\neq l'\\ k\neq k'}}e^{i(k'-k)(R_l-R_{l'})}\delta_{s_l s_{l'}} ,$$

$$e_<^2=(N-1)\left[\frac{N}{2}-1\right]-\frac{2}{N^2}\sum_{\substack{k<k_F\\ k'<k_F}}\sum_{\substack{l\neq l'\\ k\neq k'}}e^{i(k-k')(R_l-R_{l'})}\delta_{s_l s_{l'}} ,$$

$$\gamma^2=\frac{1}{N^2}\sum_{\substack{k>k_F\\ k'<k_F}}\sum_{l,l'}e^{i(k'-k)(R_l-R_{l'})}\delta_{s_l s_{l'}} ,$$

$$\beta^2=\frac{1}{N^2}\sum_{\substack{k>k_F\\ k'>k_F}}\sum_{l\neq l'}e^{i(k'-k)(R_l-R_{l'})}\delta_{s_l\bar{s}_{l'}} ,$$

$$\Delta^2=\frac{1}{N^2}\sum_{l\neq l'}\delta_{s_l\bar{s}_{l'}} ,$$

$$\mu=\frac{2}{N}\left[\sum_{k>k_F}\varepsilon_{ks}-\sum_{k<k_F}\varepsilon_{ks}\right] ,$$

where N is the number of sites, and E_0 the ground-state energy of the half-filled conduction band.

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