Incremental expansions for the ground-state energy of the two-dimensional Hubbard model

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A generalization of Faddeev's approach of the three-body problem to the many-body problem leads to the method of increments. This method was recently applied to account for the ground-state properties of Hubbard-Peierls chains [J. Malek, K. Kladko, and S. Flach, JETP Lett. **67**, 1052 (1998)]. Here we generalize this approach to two-dimensional square lattices and explicitly treat the incremental expansion up to third order. Comparing our numerical results with various other approaches (Monte Carlo, cumulant approaches) we show that incremental expansions are very efficient because good accuracy with these approaches is achieved treating lattice segments composed of eight sites only. [S0163-1829(99)50408-6]

The understanding of properties of strongly interacting fermions has been an intense topic of research for the past decade, in part due to the interest in the properties of high-temperature superconductors. As exact solutions are known only for selected integrable models, numerical methods gained importance to provide benchmarks for analytical approaches that necessarily use approximations of all kinds.

Incremental expansions have been used in quantum chemistry to account for properties of molecules and solids.[1] In a recent work[2] these methods were combined with cumulant expansions to provide a solid footing for numerical implementations. One result was that incremental expansions can be interpreted as approximative ways to solve Faddeev-like equations for the many-body problem.

To explain this in more detail, let us consider a Hamiltonian

$$H = H_0 + \sum_n H_n. \tag{1}$$

Assume that we can find the eigenenergies and eigenvectors of H_0 and of $H_0 + H_n$ for any n. Suppose further that S_n is the scattering operator associated with $H_0 + H_n$. Then Faddeev-like equations read as[2]

$$T_n = S_n \left(1 + \sum_{m \neq n} T_m \right), \quad S = \sum_n T_n, \tag{2}$$

where S is the scattering operator of the full Hamiltonian H. Assuming the S_n to be small, one obtains in lowest order $T_n = S_n$ and $S = \Sigma_n S_n$. Having the S operator one can calculate, e.g., the ground-state energy of H (for details see Ref. 2).

The ground-state energy E in zero order of the incremental expansion is equal to the ground-state energy $E^{(0)}$ of H_0. In first order we take into account the effect coming from adding one single H_n. Denote the ground-state energy of $H_0 + H_n$ by E_n. Then the first-order increment to the ground-state energy is given by $I_n^{(1)} = E_n - E^{(0)}$. This increment measures the change of adding H_n to the ground-state energy.

Summing up all increments of first order (for different n) we obtain the ground-state energy $E^{(1)}$ to first order

$$E^{(1)} = E^{(0)} + \sum_n I_n^{(1)}. \tag{3}$$

Let us now calculate the second-order increments, which take into account the simultaneous effect of adding two terms H_n and H_m. Here one has to subtract the corrections coming from adding both terms separately. Denote the ground-state energy of $(H_0 + H_n + H_m)$ with E_{nm}. Then the second-order increment is given by $I_{nm}^{(2)} = E_{nm} - I_n^{(1)} - I_m^{(1)} - E^{(0)}$. The ground-state energy to second order $E^{(2)}$ is then given by (see Chap. 5.2.3 in Ref. 1)

$$E^{(2)} = E^{(0)} + \sum_n I_n^{(1)} + \sum_{n<m} I_{nm}^{(2)}. \tag{4}$$

This procedure can be easily continued to higher orders, and the ground-state energy will be a sum over increments of all orders. It requires the exact calculation of E_{nm} when going to second order (respectively, E_{nml} when going to third order, etc.). Clearly this procedure does not imply certain topological structures induced by $\Sigma_n H_n$, so that we are not restricted to certain space dimensions if considering spatially extended systems. Note that there are many ways to split a full Hamiltonian H into a trivially solvable part H_0 and the terms H_n. Each of these ways would generate its own incremental expansions. Finally, these expansions are not restricted to the calculation of the ground-state energy only, but can also be applied to other ground-state properties and to excited states.[2]

This method was successfully applied to one-dimensional (1D) lattices.[3] There the special topology of a 1D system lead to the successive cancellation of lower order increments when proceeding to higher orders. Here we use this method to account for the ground-state energy of the two-dimensional Hubbard model on a square lattice at half filling. The Hamiltonian in dimensionless units is given by
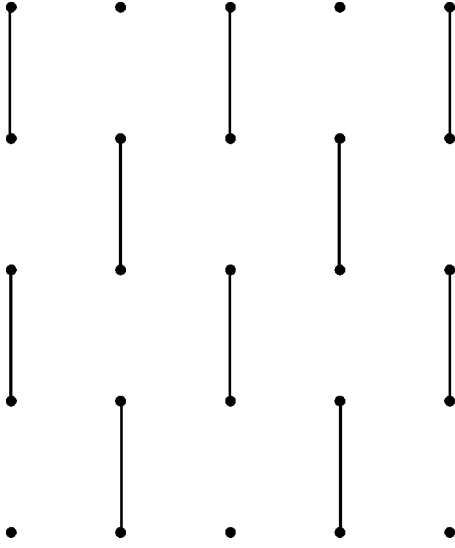
FIG. 1. Schematic representation of H_0. Circles—lattice sites, lines—bonds kept from H.

$$H_{el} = -\sum_{i,j,\sigma} (c_{i,j,\sigma}^\dagger c_{i+1,j,\sigma} + c_{i,j,\sigma}^\dagger c_{i,j+1,\sigma} + \text{H.c.})$$

$$+ U\sum_{i,j} n_{i,j,\uparrow} n_{i,j,\downarrow}. \qquad (5)$$

Here i and j are integers (which denote the x and y coordinates of the lattice points). To proceed we have to define a splitting of H_{el} into H_0 and $\Sigma_n H_n$. Here we consider H_0 as given by H_{el} when all vertical bonds and each second horizontal bond are missing (see also Fig. 1):

$$H_0 = -\sum_{i,j,\sigma} (c_{2i+j,j,\sigma}^\dagger c_{2i+j+1,j,\sigma} + \text{H.c.}) + U\sum_{i,j} n_{i,j,\uparrow} n_{i,j,\downarrow}. \qquad (6)$$

Thus H_0 is a set of horizontally aligned noninteracting dimers. Note that H_0 already contains all correlation terms of Eq. (5). The terms H_n are then the missing bonds, i.e., all vertical bonds $\Sigma_{i,j}(c_{i,j,\sigma}^\dagger c_{i,j+1,\sigma} + \text{H.c.})$ and the missing horizontal bonds $\Sigma_{i,j}(c_{2i+j-1,j,\sigma}^\dagger c_{2i+j,j,\sigma} + \text{H.c.})$.

For the sake of concreteness let us assume that our initial model Hamiltonian (5) has an even and finite number of $2N$ sites, and periodic boundary conditions. In zero order the ground-state energy E of the whole system and the energy per site ϵ are given by

$$E^{(0)} = NE(C_0), \quad \epsilon^{(0)} = \frac{1}{2}E(C_0), \qquad (7)$$

where $E(C_0)$ is the ground-state energy of the zeroth configuration C_0 that per definition is a dimer with two electrons (Fig. 2).

The first-order increment is given by adding one of the missing bonds. The ground-state energy of this case is given by sum over the ground-state energies of $N-2$ dimers (C_0) and of an open segment of two coupled dimers C_1 (see Fig. 2):
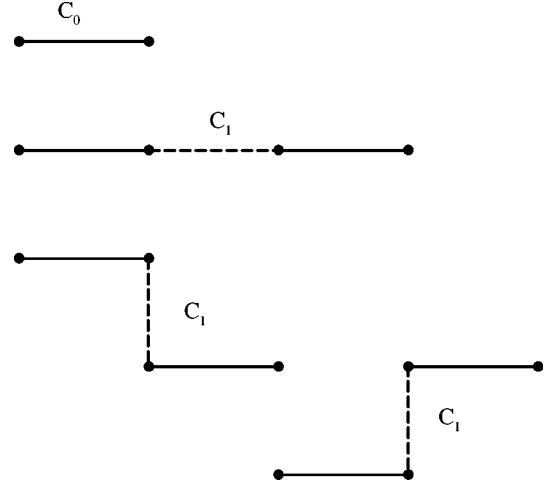

FIG. 2. Different configurations (see text).

$$I(C_1) = E(C_1) + (N-2)E(C_0) - NE(C_0)$$

$$= E(C_1) - 2E(C_0). \qquad (8)$$

We will encode all configurations of linked dimers to be considered by C_n. Note that all increments are independent of the given position of the returned bond because we assumed periodic boundary conditions. Next we need to account for the weight factor $w(C_1)$ of $I(C_1)$, i.e., the number of increments per dimer of H_0 having the same energy. It is easy to see that $w(C_1) = 3$ (all possible realizations are shown in Fig. 2). The ground-state energy in first order is then

$$E^{(1)} = E^{(0)} + 3NI(C_1) = N(3E(C_1) - 5E(C_0)),$$

$$\epsilon^{(1)} = \frac{1}{2}(3E(C_1) - 5E(C_0)). \qquad (9)$$

Already at this stage, though the considered configurations are equivalent to those of a 1D chain at the same order of incremental expansions[3] we find a difference in the energy per site due to the increased number of nearest neighbors of the 2D lattice as compared to the 1D case.

In second order we have to add two of the missing bonds. Nonzero contributions come from cases when the two returned bonds are linked.[2] Then we have two nonzero configurations C_2 (open chain with six sites) and C_3 (which is already incorporating topological effects of the 2D system) in this order (see Fig. 3). Their weight factors are $w(C_2) = 9$ and $w(C_3) = 6$. The corresponding increments are

$$I(C_2) = E(C_2) - 3E(C_0) - 2I(C_1)$$

$$= E(C_2) - 2E(C_1) + E(C_0), \qquad (10)$$

$$I(C_3) = E(C_3) - 3E(C_0) - 2I(C_1)$$

$$= E(C_3) - 2E(C_1) + E(C_0). \qquad (11)$$

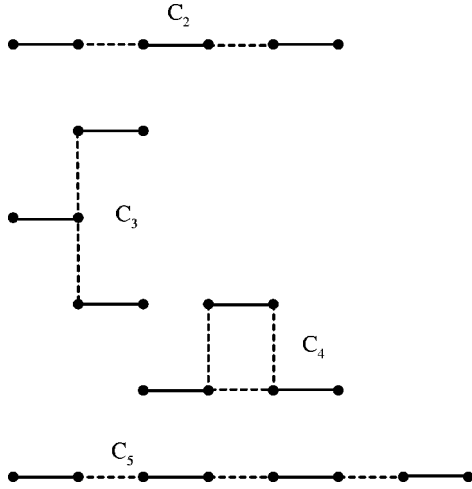The ground-state energy can be evaluated according to Eq. (4):

FIG. 3. Same as Fig. 2.

$$\epsilon^{(2)} = \frac{1}{2}E(C_0) + \frac{3}{2}I(C_1) + \frac{9}{2}I(C_2) + 6I(C_3)$$

$$= 5E(C_0) - 13.5E(C_1) + 4.5E(C_2) + 3E(C_3). \quad (12)$$

Since the topology of the configurations starts to be different from those appearing in a 1D system[3] no trivial cancellation of lower order increments takes place anymore.

In third order we add three missing bonds (again only configurations when all three returned bonds are linked do contribute). We obtain six different configurations $C_4, C_5, C_6, C_7, C_8, C_9$ with corresponding weight factors 2,27,2,10,18,32. They are shown in Figs. 3 and 4. The corresponding increments are

$$I(C_4) = E(C_4) - I(C_2) - 2I(C_3) - 3I(C_1) - 3E(C_0), \quad (13)$$

$$I(C_5) = E(C_5) - 2I(C_2) - 3I(C_1) - 4E(C_0), \quad (14)$$

$$I(C_6) = E(C_6) - 3I(C_3) - 3I(C_1) - 4E(C_0), \quad (15)$$

$$I(C_7) = E(C_7) - 2I(C_3) - 3I(C_1) - 4E(C_0), \quad (16)$$

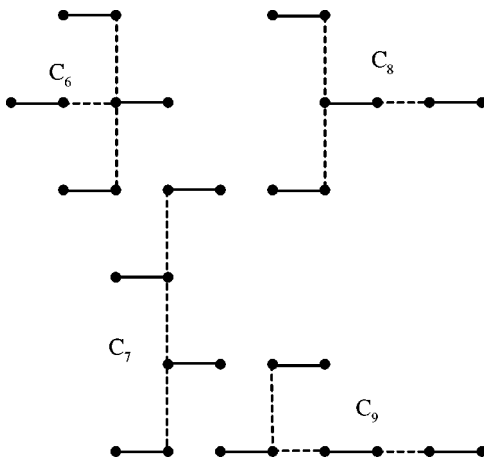$$I(C_8) = E(C_8) - I(C_3) - 2I(C_2) - 3I(C_1) - 4E(C_0), \quad (17)$$
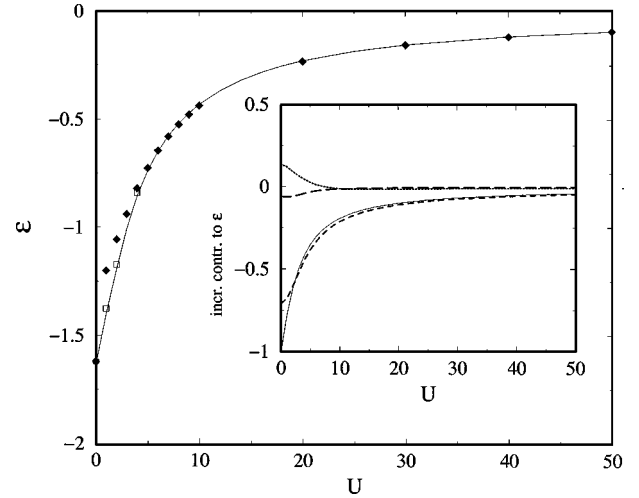

FIG. 4. Same as Fig. 2.

FIG. 5. ϵ versus U. Solid line—result from third incremental order; filled circle—exact value at $U=0$; open squares—QMC results (Ref. 4); filled diamonds—projection operator results (Ref. 5). Inset: Dependence of incremental contributions to ϵ on U. Solid line—zeroth order; thick dashed line—first order; thick long-dashed line—second order; dotted line—third order.

$$I(C_9) = E(C_9) - I(C_2) - I(C_3) - 3I(C_1) - 4E(C_0). \quad (18)$$

It is too lengthy to explicitly write down the formula for the ground-state energy. In the following we will present the results of numerical calculations.

We use a Lanczos algorithm to compute the ground-state energies of our considered configurations. In Fig. 5 we show the dependence of the ground-state energy per site ϵ on the interaction parameter U in third order of the incremental expansion. In the inset of Fig. 5 we show the U dependence of the different incremental contributions. We find that the contributions coming from second and third order are small compared to the zeroth and first order. For free electrons $U=0$ we compare ϵ for zeroth, first, second, and third orders: -1; -1.708204; -1.768700; -1.6335775 with the exact number $\epsilon(U=0) = -1.621139$ (see also Table I and Fig. 5). This gives a relative error of only 0.8%! For $U=1,2,4$ we compare ϵ in third order in Table I with quantum Monte Carlo (QMC) calculations of Moreo *et al.*,[4] where lattices with sizes up to 16×16 were used and extrapolations were carried out. The relative difference (Table I) is less than 2%. Note that the slight increase in the relative error with increasing U at least partially has to be attributed to the circumstance that the QMC calculations become less exact with increasing U. Also in Fig. 5 the results of Polatsek and Becker on related projection operator techniques using cu-

TABLE I. Comparison of ϵ in third order with QMC results and exact value for $U=0$.

U	ϵ (Ref.)	ϵ (third order inc.)
0	-1.621 (exact)	-1.634
1	-1.376 (4)	-1.400
2	-1.172 (4)	-1.191
4	-0.841 (4)	-0.856
∞ (Heisenberg)	-0.669 (6)	-0.670

mulants are shown.[5] These calculations take spin flips up to second order and charge fluctuations up to second order (in terms of our notations) into account. The agreement is very good in a broad range of U values. The exception is the limit of small U, where the projection technique becomes less accurate. Finally, for large U the Hubbard model transforms into the Heisenberg model. Doing the same calculations for the Heisenberg model with $J=1$ we compare ϵ for zeroth, first, second, and third orders: -0.375; -0.5490375; -0.578994; -0.6695330 with the results of QMC calculations of the ground-state energy of the Heisenberg model $\epsilon \approx -0.669$ by Runge[6] (see also Refs. 5 and 7–9 with similar results). The relative difference is less than 0.08% (see also Table I). To conclude this part, we emphasize that our results yield a high precision (relative differences of the order of 2% and less) in the whole U range, which has not been achieved by any of the other methods discussed.

Let us emphasize that the presented method is not just a clever way of making finite size extrapolations. To show that, we consider the two-dimensional antiferromagnetic Ising model $H = \Sigma_{ij} S_i^z S_j^z$ on a square lattice with spin 1/2. The ground-state energy per site is given by $-1/2$, which is simply the result of each site having two bonds, each bond contributing with an energy of $-1/4$. Any finite size calculation of this energy would deviate from the exact value, because it would involve the energy of spins at the boundary of the finite size cluster, where the number of contributing bonds per site is less than 2. However, it is an easy task to check, that our method gives $E(C_0) = -1/4$, $I(C_1) = -1/4$, $I(C_n) = 0$ for $n \neq 0,1$. Thus our expansion terminates after the first order, and in this order we obtain precisely $\epsilon = -1/2$. This should make clear that incremental expansions are at any stage yielding results for the infinite lattice.

Using exact diagonalizations we could extend the calculations even further up to sixth order, i.e., up to adding six missing bonds. This needs a careful classification of all contributing configurations and their weight factors. We are currently working on this project. Notice the extremely high precision that we achieve already in 3D order, where the largest systems we have to deal with consist of eight sites. Without any extrapolation we obtain a precision which, e.g., in QMC is achieved by considering systems with size up to $16 \times 16 = 256$ sites and additional extrapolations (cf. Fig. 5 in Ref. 10). The reason for this is the fact that we use a scheme that at each level describes an infinite system, and accounts for the important topological structures through the weight factors. This appears to be much better than just to consider a finite lattice with a certain size. Having the ground-state energy with that accuracy, we plan next to account for the dimerization of a two-dimensional Hubbard-Peierls system. Work is in progress.

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