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

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Abstract

A generalization of Faddeev’s approach of the 3-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 (JETP Letters 67 (1998) 1052). 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 those approaches is achieved treating lattice segments composed of 8 sites only.
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 which 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 N-body problem.

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

\[ H = H_0 + \sum_n H_n , \]  

(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 \[2\]

\[ T_n = S_n (1 + \sum_{m \neq n} T_j) , \quad S = \sum_n T_n , \]  

(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 \( S = \sum_n S_n \). Having the \( S \) operator one can calculate e.g. the ground state energy of \( H \) (for details see \[2\]).

The ground state energy \( E \) in zero order of the incremental expansion equals 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

\[ E^{(1)} = E^{(0)} + \sum_n I_n^{(1)} . \]  

(3)
Let us now calculate the second order increments, which are taking 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 Chapter 5.2.3 in \[1\])

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

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 \(\sum_n H_n\), 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 be also applied to other ground state properties and to excited states \[2\].

This method was successfully applied to one-dimensional 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

\[
H_{el} = -\sum_{i,j,\sigma}(c^\dagger_{i,j,\sigma}c_{i+1,j,\sigma} + c^\dagger_{i,j,\sigma}c_{i+1,j,\sigma} + h.c.) + U \sum_{i,j} n_{i,j,\uparrow} n_{i,j,\downarrow} .
\]

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 \(\sum_n H_n\). 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):

\[
H_0 = -\sum_{i,j,\sigma}(c^\dagger_{2i+j,j,\sigma}c_{2i+j+1,j,\sigma} + h.c.) + U \sum_{i,j} n_{i,j,\uparrow} n_{i,j,\downarrow} .
\]
Thus $H_0$ is a set of horizontally aligned noninteracting dimers. Note that $H_0$ already contains all correlation terms of (5). The terms $H_n$ are then the missing bonds i.e. all vertical bonds $\sum_{i,j}(c_{i,j,\sigma}^\dagger c_{i,j+1,\sigma} + h.c.)$ and the missing horizontal bonds $\sum_{i,j}(c_{2i+j-1,j,\sigma}^\dagger c_{2i+j,j,\sigma} + h.c.)$.

For 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 $\epsilon$ are given by

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

where $E(C_0)$ is the ground state energy of the 0th configuration $C_0$ which 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):

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

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

$$E^{(1)} = E^{(0)} + 3NI(C_1) = N(3E(C_1) - 5E(C_0)), \quad \epsilon^{(1)} = \frac{1}{2}(3E(C_1) - 5E(C_0)).$$

Already at this stage, though the considered configurations are equivalent to those of a 1d chain at the same order of incremental expansions [4] we find a difference in the energy per site due to the increased number of nearest neighbours 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

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

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

The ground state energy can be evaluated according to [4]:

$$\epsilon^{(2)} = \frac{1}{2} E(C_0) + \frac{3}{2} I(C_1) + \frac{9}{2} I(C_2) + 6I(C_3) = 5E(C_0) - 13.5E(C_1) + 4.5E(C_2) + 3E(C_3) .$$

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.3,4. The corresponding increments are

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

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

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

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

$$I(C_8) = E(C_8) - I(C_3) - 2I(C_2) - 3I(C_1) - 4E(C_0)$$

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

It is too tedious 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 Lancosz 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 $\epsilon$ 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 2nd and 3rd order are small compared to the 0th and 1st order. For free electrons $U = 0$ we compare $\epsilon$ for 0th, 1st, 2nd and 3rd orders $-1; -1.708204; -1.768700; -1.6335775$ with the exact number $\epsilon(U = 0) = -1.621139$ (see also Table 1 and Fig.5). This gives a relative error of only 0.8% ! For $U = 1, 2, 4$ we compare $\epsilon$ in 3rd order in Table 1 with quantum Monte Carlo (QMC) calculations of Moreo et al [4], where lattices with sizes up to $16 \times 16$ were used and extrapolations were carried out. The relative difference (Table 1) 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 cumulants 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 $\epsilon$ for 0th, 1st, 2nd and 3rd 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 [6], [7], [8] and [9] with similar results). The relative difference is less than 0.08% (see also Table 1). 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 $H = \sum_{ij} S^z_i S^z_j$ 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 6th 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 which we achieve already in 3d order, where the largest systems we have to deal with consist of 8 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 [10]). The reason for this is the fact that we use a scheme which 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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TABLE 1.

Comparison of $\epsilon$ from 3rd order increments with QMC results and exact value for $U = 0$.

| $U$      | $\epsilon$ (ref)         | $\epsilon$ (3rd 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                       |
| $\infty$ (Heisenberg) | -0.669 (3)   | -0.670                       |
FIGURE CAPTIONS

Fig.1
Schematic representation of $H_0$. Circles - lattice sites, lines - bonds kept from $H$.

Fig.2
Different configurations (see text).

Fig.3
Same as Fig.2

Fig.4
Same as Fig.2

Fig.5
$\epsilon$ versus $U$. Solid line - result from third incremental order; filled circle - exact value at $U = 0$; open squares - QMC results [3]; filled diamonds - projection operator results [3].
Inset: Dependence of incremental contributions to $\epsilon$ on $U$. Solid line - 0th order; thick dashed line - 1st order; thick long dashed line - 2nd order; dotted line - 3rd order.
Fig. 1
Fig. 2

$C_0$

$C_1$

$C_1$

$C_1$
Fig. 4

$C_6$  

$C_7$  

$C_8$  

$C_9$
Fig. 5 Malek et al.