Cumulant $t$-expansion for strongly correlated fermions

A. K. Zhuravlev
Institute of Metal Physics, 620990 Ekaterinburg, Russia
(Dated: November 7, 2018)

A systematic nonperturbative scheme is implemented to calculate the ground state energy for a wide class of strongly correlated fermion models. The scheme includes: (a) method of automatic calculations of the cumulants of the model Hamiltonian; (b) method of the ground state energy calculation from these cumulants using the $t$-expansion proposed by Horn and Weinstein [Phys. Rev. D 30, 1256 (1984)] with new procedure of its extrapolation to $t \to \infty$. As an example of application of the method all cumulants up to the 8-th order for spinless fermion model are calculated exactly, and converging sequences of approximations to the ground state energy are obtained for one-, two- and three-dimensional versions of the model.

PACS numbers: 05.30.Fk, 71.10.Fd, 71.15.-m

I. INTRODUCTION

The problem of strongly correlated quantum many-body systems is one of the most complicated in theoretical physics. With the exception of a few of simplified models this problem cannot be solved analytically, so that one must resort to numerical methods. But here a researcher is faced with serious difficulties. For example, exact diagonalization runs into the exponential growth of the Hilbert space dimension with increasing size of the system and therefore is limited to small clusters, even when using the Lanczos algorithm. A more sophisticated Density-Matrix Renormalization Group technique with high-energy states truncation gives excellent results for the ground state energy of one-dimensional Fermi systems, but has its own limitation when applied to two- and three-dimensional cases. Quantum Monte Carlo method can potentially handle larger systems. However, the method works poorly at low temperatures for fermion systems because of the so called “minus-sign” problem.

As an alternative, a certain interest in the construction of regular expansions still exists. The attractive feature of such alternative is the relative simplicity of calculation of terms in the expansion. Unfortunately, the series expansions in powers of the coupling constants usually diverge. However, there are regular expansion methods which are not reduced to power expansion in coupling constant. For example, high-temperature expansion is that one worth to mention.

Another one is the so called $t$-expansion, which we describe briefly in what follows. Given a Hamiltonian $\hat{H}$ and an initial state $|\phi_0\rangle$, let us define the moments

$$\mu_m = \langle \phi_0 | \hat{H}^m | \phi_0 \rangle$$

(|$\phi_0$) is normalized to unity) and introduce auxiliary function

$$E(t) = \frac{\langle \phi_0 | \hat{H} e^{-\hat{H}_t} | \phi_0 \rangle}{\langle \phi_0 | e^{-\hat{H}_t} | \phi_0 \rangle}$$

which can be written as a power series in the parameter $t$:

$$E(t) = \sum_{m=0}^{\infty} \frac{I_{m+1} (-t)^m}{m!} ,$$

where

$$I_{m+1} = \mu_{m+1} - \sum_{p=0}^{m-1} \binom{m}{p} I_{p+1} \mu_{m-p}$$

are the cumulants (note that in the $t$-expansion the values $I_m$ were named “connected moments”). Then

$$E_0 = \lim_{t \to \infty} E(t)$$

is the minimal eigenvalue of the Schrödinger equation

$$\hat{H} |\psi_0\rangle = E_0 |\psi_0\rangle$$

provided that $\langle \psi_0 | \phi_0 \rangle \neq 0$ (see for proof).

There were attempts to use $t$-expansion in lattice gauge theory, quantum chromodynamics, quantum chemistry. In condensed matter physics $t$-expansion was applied to the square lattice Heisenberg antiferromagnet. For the models of interacting electrons on a lattice this method is not used mainly for two reasons: 1) it is difficult to calculate cumulants $I_m$ for any realistic model, 2) it is not easy to calculate the limit having the finite number of known cumulants. In this paper we present a solution to both of these problems and test it for the spinless fermion model which is a typical example of strongly correlated fermion models.

II. CALCULATION OF THE CUMULANTS

The Hamiltonian of this model reads

$$\hat{H} = \hat{W} + \hat{V} , \quad \hat{W} = -w \sum_{i>j} c_i^\dagger c_j + c_j^\dagger c_i , \quad \hat{V} = v \sum_{i>j} c_i^\dagger c_j c_j^\dagger c_i$$

with $i$ and $j$ being nearest neighbor lattice sites.
The one-dimensional spinless fermion model is equivalent to the exactly solvable spin-1/2 XXZ model. Therefore, the model is in one dimension is often used to test new methods of calculations (see, e.g., [2]). Note that for the half-filled case of the model the metal-insulator transition takes place with the appearance of the gap in the energy spectrum at $v > 2w$.

If the initial wavefunction $|\phi_0\rangle$ has the form

$$
|\phi_0\rangle = \prod_i c_i^\dagger |0\rangle
$$

($|0\rangle$ is the state without fermions, $l$ runs over some set of the lattice sites) then many-operator average included in cumulant $I_n$ can be calculated using Wick’s pairing technique. We have to

1) connect each creation operator $c_i^\dagger$ with one of the annihilation operators $c_j$ with lines by all the ways possible, 2) for each way of the connection assign a term with factor $(-1)^P$, where $P$ is the number of connecting lines intersections, 3) replace each connected pair of operators $c_i^\dagger$ and $c_j$ (or $c_i$ and $c_j^\dagger$) by the average $\langle c_i^\dagger c_j \rangle_0$ (or $\langle c_i c_j^\dagger \rangle_0$), where we introduced the notation $(\ldots)_0 = \langle \phi_0 | \ldots | \phi_0 \rangle$.

For example, the calculation of 4-operator average is

$$
\langle c_i^\dagger c_j c_k^\dagger c_l \rangle_0 = \langle c_i^\dagger c_j \rangle_0 \langle c_k^\dagger c_l \rangle_0 + \langle c_i^\dagger c_j \rangle_0 \langle c_k c_l^\dagger \rangle_0 + \langle c_i c_j^\dagger \rangle_0 \langle c_k^\dagger c_l \rangle_0 + \langle c_i c_j^\dagger \rangle_0 \langle c_k c_l^\dagger \rangle_0
$$

where $n_i = 1$ if $i$-th site in $|\phi_0\rangle$ is filled, and $n_i = 0$ if the site is an empty one. Thus each average can be computed easily, but there are too many of them to perform all the calculations manually. To complete the task the symbolic manipulation computer program was written that performs these calculations.

To be certain let us consider the one-dimensional half-filled case with the initial state $|\phi_0\rangle = |10101010...10\rangle$. For this state $V|\phi_0\rangle = 0$, so that the terms included in $\langle \hat{H}^n \rangle_0$ which begin with or end with the operator $\hat{V}$ vanish altogether. Therefore one obtains simpler expressions for the moments $\mu_n$:

$$
\mu_1 = \langle \hat{H} \rangle_0 = \langle \hat{W} \rangle_0 ,
$$

$$
\mu_2 = \langle \hat{H}^2 \rangle_0 = \langle \hat{W} \hat{W} \rangle_0 ,
$$

$$
\mu_3 = \langle \hat{H}^3 \rangle_0 = \langle \hat{W} \hat{W} \hat{W} \rangle_0 + \langle \hat{W} \hat{V} \hat{W} \rangle_0 , \ldots
$$

Substituting (10) into (4) we obtain compact expressions for the cumulants

$$
I_1 = \langle \hat{W} \rangle_0 ,
$$

$$
I_2 = \langle \hat{W} \hat{W} \rangle_0 ,
$$

$$
I_3 = \langle \hat{W} \hat{W} \hat{W} \rangle_0 + \langle \hat{W} \hat{V} \hat{W} \rangle_0 , \ldots
$$

where the index “c” means that only connected terms give contribution in pairings like (10), i.e. those in which isolated group of operators $\hat{W}$ and $\hat{V}$ are absent.

Substituting the expressions (7) for $\hat{W}$ and $\hat{V}$ into (11), using Wick’s pairing technique and performing necessary analytical calculations with the help of the above-mentioned computer program, we obtain the final expressions for cumulants of the half-filled one-dimensional spinless fermion model:

$$
I_1 = 0 ,
$$

$$
I_2 = -86w^4 v^2 + 2w^2 v^4 N ,
$$

$$
I_3 = -28w^4 v + 2w^2 v^3 N ,
$$

$$
I_4 = -160w^6 - 86w^4 v^2 + 2w^2 v^4 N ,
$$

$$
I_5 = (1704w^8v - 220w^6v^3 + w^2v^5) N ,
$$

$$
I_6 = -9520w^8 + 10736w^6v^2 - 510w^4v^4 + w^2v^6 N
$$

where $N$ is the number of lattice sites. The number of cumulants which could be computed is limited by a computer power only.

### III. CALCULATION OF THE LIMIT $E(t \to \infty)$

The next step is the calculation of the limit (13). In order to calculate this limit one must know all the cumulants, which is impossible for any real system. All that we know about the function $E(t)$ is its finite power series

$$
E(t) = \sum_{m=0}^{M+1} \frac{I_{m+1}}{m!} (-t)^m
$$

and the following information: 1) the function $E(t)$ is a monotonically decreasing one since the derivative of (2) is the negative of the expectation value of the positive operator $(\hat{H} - \langle \hat{H} \rangle)^2$, i.e. $\frac{dE}{dt} < 0$; 2) $E(t)$ rapidly goes to a constant, hence $\frac{dE}{dt}$ goes to zero as $t$ goes to infinity. The

![FIG. 1: The ground state energy density for one-dimensional half-filled spinless fermion model calculated by different methods using the cumulants up to $I_7$.](image-url)
\[ E(t) = \int_0^\infty E'(t)dt = E(\infty) - E(0) = E_0 - I_1 \]

where \( E'(t) = \frac{dE(t)}{dt} \), and we have to find the best way to interpolate the function \( E'(t) \) between its known values \( E'(0) = -I_2 \) and \( E'(\infty) = 0 \).

Let us expand the initial state \( |\phi_0\rangle \) in terms of the eigenfunctions of the Hamiltonian as

\[ |\phi_0\rangle = \sum_{n=0}^{\infty} \sqrt{b_n}|\psi_n\rangle \]

with \( \hat{H}|\psi_n\rangle = E_n|\psi_n\rangle \). Then the function \( E(t) \) can be rewritten as

\[ E(t) = \frac{\int_{E_0}^{E_{\max}} E e^{-Et}\rho(E)dE}{\int_{E_0}^{E_{\max}} e^{-Et}\rho(E)dE} \]

where \( \rho(E) = \sum_n b_n\delta(E - E_n) \). Direct differentiation of \( E'(t) \) shows that the asymptotic behavior of the function \( E'(t) \) at \( t \to \infty \) depends on the features of the eigenvalue spectrum. Let us consider the two limiting cases: 1) for continuous spectrum with \( \rho(E) = \text{const} \ E'(t) \sim -1/t^2 \); 2) for discrete spectrum \( E'(t) \sim -e^{-\Delta t} \), where \( \Delta \) is the gap between the ground state energy \( E_0 \) and the first excited state energy \( E_1 \).

Now let us consider the function \( Q(t) \equiv -I_2/E'(t) \). Its asymptotic behavior must be between \( t^2 \) and \( e^{\Delta t} \). Given the cumulants from \( I_1 \) to \( I_{M+2} \), calculating \( 0/M \) Padé approximant for \( E'(t) \) we obtain the series expansion for function \( Q(t) \) up to order \( M \):

\[ Q_M(t) = 1 + q_1 t + q_2 t^2 + \ldots + q_M t^M. \]

If the values \( q_m \) are close to the coefficients of expansion of the exponential, i.e. there is a good fit to the dependence

\[ q_m \approx \frac{\alpha^m}{m!} \ (\alpha > 0) \]

(see Fig 2) there is a reason to assume that \( Q(t) \sim e^{\alpha t} \) and take into account the contribution by Kummer’s series transformation method. Namely, let us introduce

\[ \alpha = \frac{1}{M} \sum_{m=1}^{M} (m!q_m)^{1/m} \]

and replace \( Q_M(t) \) by \( \tilde{Q}_M(t) \):

\[ \tilde{Q}_M(t) = Q_M(t) + e^{\alpha t} - \sum_{m=0}^{M} \frac{\alpha^m}{m!} t^m \]

where the first \( M \) terms of the series for \( \tilde{Q}_M(t) \) coincide with \( Q_M(t) \). Then an expression for the approximate ground state energy is

\[ E_0(I_{M+2}) = I_1 - \int_0^{\infty} \frac{I_2}{Q_M(t)} dt \]

The appearance of negative \( q_m \) in (17) should be considered as an indication that the function \( Q(t) \) has no an exponential asymptotics. Therefore, it has the power asymptotics. Here it is reasonable to use the Padé approximants for \( Q(t) \) (or \( E'(t) \)). For the integral in (14) is finite we can use for \( E'(t) \) only approximants like \( 0/M \ldots [L/M - L] \ldots \), where \( M - L \gg L + 2 \). Since \( E'(t) \) is always negative we have to control that this property holds for the Padé approximants. If some approximant has alternating-sign at certain values of \( L \) then we will exclude it from consideration. For each of the remaining proper approximants we calculate the ground state energy \( E_0 \) according to (14). And if the number of proper approximants is more than one, then we carry out averaging over the energies calculated.

The new extrapolation method described above we call adapted derivative (AD) method.

![Figure 2](image-url) The quantity \( \alpha_m \equiv \text{sgn}(q_m)(m!q_m)^{1/m} \) for one-dimensional half-filled spinless fermion model. The right column shows the exact value of the gap \( \Delta \) in the thermodynamical limit.
As one can see the estimation for the ground state energy converges to its exact value with increasing of the number of the cumulants known. The new AD-method radically accelerates the convergence rate compared to D-Padé approximation for large \(v/w\), that is, where there is a large gap \(\Delta\) in the energy spectrum, despite the fact that \(\alpha \leq 1\) is only a rough estimate for \(\Delta\) (see Fig.3). For \(v \lesssim w\) the accuracy of the AD-method is comparable to the accuracy of the D-Padé method. The last case is the most difficult for the method provided the particle-hole alternating ordered initial state \(\ket{\phi_0}\) is chosen.

### IV. SQUARE AND SIMPLE CUBIC LATTICES

Now let us discuss two- and three-dimensional spinless fermion models, where the exact solutions are not known, except for a case of non-interacting particles \(v = 0\). For half-filled spinless fermion model on a square lattice with chessboard ordered initial state \(\ket{\phi_0}\) the cumulants are:

\[
I_1 = 0, \quad I_2 = 2w^2N, \quad I_3 = 6w^2vN,
I_4 = (-36w^4 + 18w^2v^2)N,
I_5 = (-488w^4v + 54w^2v^3)N,
I_6 = (3200w^6 - 4516w^4v^2 + 162w^2v^4)N,
I_7 = (96304w^6v - 35576w^4v^3 + 486w^2v^5)N,
I_8 = (-664000w^8 + 1794464w^6v^2 - 257044w^4v^4 + 1458w^2v^6)N.
\]

The results for the ground state energy density is presented in Fig.3 and Tab.II.

For half-filled spinless fermion model on the simple cubic lattice with “three-dimensional chessboard” ordered initial state \(\ket{\phi_0}\) the cumulants are:

\[
I_1 = 0, \quad I_2 = 3w^2N, \quad I_3 = 15w^2vN,
I_4 = (-90w^4 + 75w^2v^2)N,
\]

\[
I_5 = (-2052w^4v + 375w^2v^3)N,
I_6 = (14880w^6 - 32058w^4v^2 + 1875w^2v^4)N,
I_7 = (744600w^8v - 427572w^6v^3 + 9375w^2v^5)N,
I_8 = (-6083280w^8v + 23234064w^6v^2 - 5240898w^4v^4 + 46875w^2v^6)N.
\]

The results for the ground state energy density is presented in Fig.3 and Tab.II.

In both cases, the approximations sequence converge, behaving similarly to the one-dimensional case.

### V. CONCLUSIONS

As we have seen, the present method yields converging sequence of approximations to the ground state energy of a typical strong-correlated many-fermion model. Seemingly, the sequence of approximations will converge for
TABLE III: The sequences of $[0/M]$D-Padé and AD approximations to the ground state energy density $E_0/(Nw)$ for half-filled spinless fermion model on simple cubic lattice using the cumulants up to $I_{M+2}$

| $v/w$ | 0    | 2    | 5    | 10   | 20   |
|-------|------|------|------|------|------|
| DP($I_4$) | -1.216734 | -0.427777 | -0.185303 | -0.093840 | -0.047073 |
| DP($I_5$) | -1.216734 | -0.317453 | -0.137238 | -0.069500 | -0.034864 |
| DP($I_6$) | -0.970781 | -0.290241 | -0.125303 | -0.063438 | -0.031820 |
| DP($I_7$) | -0.970781 | -0.281633 | -0.121129 | -0.061306 | -0.030749 |
| DP($I_8$) | -0.991937 | -0.278155 | -0.119448 | -0.060446 | -0.030317 |
| AD($I_4$) | -1.015876 | -0.280232 | -0.118592 | -0.059821 | -0.029978 |
| AD($I_5$) | -1.129247 | -0.275983 | -0.118229 | -0.059773 | -0.029972 |
| AD($I_6$) | -0.963441 | -0.274673 | -0.118121 | -0.059759 | -0.029970 |
| AD($I_7$) | -0.970781 | -0.274901 | -0.118099 | -0.059756 | -0.0299692 |
| AD($I_8$) | -0.995160 | -0.275095 | -0.118096 | -0.059755 | -0.0299691 |
| exact    | -1.002420 |           |           |       |      |

any Hamiltonian whose moments (1) are finite. The generalization of the method to the case of real electrons with spin is very simple: one needs to pair only the operators with the same spin indices in the formulas like (9). Therefore the method is applicable to real many-electron problems in condensed matter physics and quantum chemistry. The method is of interest for researchers because it gives a systematic approach to physical problems with strong interaction, which does not require the smallness of the interaction. The AD-method which we introduce to calculate the limit $E(t \to \infty)$ can be useful in the traditional areas of the $t$-expansion application, like the lattice gauge theory and quantum chromodynamics.

The research was carried out within the state assignment of FASO of Russia (theme “Electron” No. 01201463326).

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* Electronic address: zhuravlev@imp.uran.ru

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