Generalized Quantum Monte Carlo Algorithm in Eigen Basis

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Abstract. New generalized continuous-time quantum Monte Carlo algorithm is developed. The algorithm is absolutely universal in the sense that it allows to calculate models specified in an arbitrary basis (in the basis of occupation numbers; in the momentum representation; in the basis of the eigenfunctions of small clusters into which the entire system is divided, or in any other basis): the algorithm requires only the specification of the matrix elements between the basis functions defined in a convenient basis. The implemented algorithm is applied to one-dimensional Hubbard model.

1. Introduction

Exact numerical methods are often the only way to obtain the answer for complex systems which a modern experiment deals with; it is caused by the lack of expansion parameters in interacting systems that does not allow carrying out analytical calculations with necessary accuracy. As far as quantum matter is concerned, Monte Carlo algorithms are among the most powerful tools for studying of such systems [1, 2]. There is a vast number of modifications of quantum Monte Carlo algorithms depending on problems being addressed. Among the most used are determinant method for discrete [3] and continuous time [4]; variational Monte Carlo for zero-temperature studies [5]; diagrammatic techniques based on Matsubara Green’s function decomposition [6, 7]; continuous-time world line (CTWL) algorithms [8]. The last ones are based on interaction representation of the partition function and are free from the systematic error associated with Trotter decomposition. CTWL algorithms were successfully implemented to study lattice systems of various size, dimensions, and statistics.

Although being rather universal in its formulation, CTWL algorithm requires certain variations which depend on the problem under study (such as the choice of an appropriate basis functions, the set of configuration updates, etc.).

The aim of this work is to create an algorithm that will be “universal”, i.e. it will allow calculation of lattice models defined in an arbitrary basis (in the basis of occupation numbers, in the momentum representation, in the basis of the eigenfunctions of the small clusters to which the whole system is divided, or in any other basis). Such an algorithm will require only the specification of matrix elements between the basis functions given in a convenient basis. In this formulation, the algorithm can be equally easily applied to multi-orbital models of any complexity.

This article continues a series of works by authors on the development of the CTWL algorithm in relation to various strongly correlated systems [9-13].
2. Method

In its most general form, CTWL algorithm is applicable to systems with the following Hamiltonian:

\[ H = \sum_{k\ell n_2 n_3} t_{k\ell}^{n_1 n_2 n_3 n_4} \left( A_k^{n_1 n_2} A_\ell^{n_3 n_4} + h. c. \right) + \sum_{k\ell n_2 n_4} U_{k\ell}^{n_1 n_2 n_3 n_4} + \sum_{kn} U_k^{n_1 n_2} \tilde{M}_k^{n_3 n_4} \]

\[ + \sum_{k\ell n_1 n_2} U_k^{n_1 n_2} (\tilde{A}_k^{n_1 n_2} + h. c.) + \sum_{k\ell n_1 n_2} \overline{C}_k^{n_1 n_2} + \sum_{k\ell n_1 n_2 n_3} \overline{D}_k^{n_1 n_2 n_3} \tilde{N}_k^{n_3} (\tilde{A}_k^{n_1 n_2} + h. c.), \]

where indexes \( k, \ell \) count the sites of the discrete basis; \( n_1, n_2, \ldots \) are quantum states of each site; operators \( \tilde{A}_k^{n_1 n_2} \) describe the transition of site \( k \) from state \( n_1 \) to state \( n_2 \); \( \tilde{N}_k^{n_1 n_2} \) and \( \overline{M}_k^{n_1 n_2} \) are diagonal operators in the chosen basis. All parameters of the Hamiltonian (1) characterizing hopping amplitudes \( t \), diagonal interparticle interactions \( U \) and responses to external transverse \((B, D)\), and longitudinal \((C)\) fields can be unique for each state and site, and also take into account all features of the statistics (Bose, Fermi, or spin). The action of operators on basis functions leads either to a transition to new states for operators that are non-diagonal for a given representation or a state remains unchanged in the case of diagonal operators:

\[ \tilde{A}_k^{n_1 n_2} \left| \ldots n_1^k \ldots \right\rangle \sim \left| \ldots n_2^k \ldots \right\rangle; \]

\[ \tilde{N}_k^{n_1 n_2} \left| \ldots n_1^k \ldots \right\rangle \sim \left| \ldots n_1^k \ldots \right\rangle; \]

\[ \overline{M}_k^{n_1 n_2} \left| \ldots n_1^k \ldots \right\rangle \sim \left| \ldots n_2^k \ldots \right\rangle. \]

Here we consider the case when the site states \( n^k \) are the eigenstates of some part of Hamiltonian (1) corresponding, e.g., to a small cluster of the initial lattice on which (1) is defined. In this situation, the whole Hamiltonian is decomposed into the sum of inter- and intra-cluster operators,

\[ H = \sum_{i=1}^{N_c} H_{\text{inter}} + \sum_{i=1}^{N_c} H_{\text{intra}}, \]

where \( N_c \) is the number of clusters in the system. Each cluster should be small enough to be solvable by, e.g., exact diagonalization technique. Possible decompositions of one- and two-dimensional lattices are shown in figure 1.

**Figure 1.** One- and two-dimensional lattice models decomposed as sums of small clusters.

The basis functions \( \varphi \) in this representation are the eigenfunctions of each cluster, i.e. the eigenfunctions of \( H_{\text{intra}} \):

\[ \varphi: H_{\text{intra}} \varphi_i = \epsilon_i \varphi_i, \quad i = 1, \ldots, 4^L. \]
Here \( L \) is the number of sites in each cluster, and a spinful fermion model is assumed. The state of the whole system is

\[
\Phi = |\varphi_1\rangle \otimes |\varphi_2\rangle \otimes \ldots \otimes |\varphi_N\rangle.
\]  

(5)

\( H_{\text{intra}} \), which is typically specified in the occupation number representation, transforms the basis functions in a general way,

\[
H_{\text{intra}} |\varphi_\alpha\rangle = \sum_{\alpha'} c_{\alpha'} |\varphi_{\alpha'}\rangle,
\]  

(6)

while \( H_{\text{inter}} \), in its simplest form, changes the states of two adjacent clusters (Fig. 2):

\[
H_{\text{inter}}(|\varphi_\alpha\rangle \otimes |\varphi_\beta\rangle) = \sum_{\alpha',\beta'} c_{\alpha'\beta'} (|\varphi_{\alpha'}\rangle \otimes |\varphi_{\beta'}\rangle).
\]  

(7)

**Figure 2.** Action of \( H_{\text{intra}} \) and \( H_{\text{inter}} \) on basis functions.

The matrix elements \( c_\alpha \) and \( c_{\alpha\beta} \) in (6) and (7) serve as input parameters for Monte Carlo scheme. When accounting for all matrix elements, the algorithm is absolutely exact. However, the number of matrix elements is proportional to the square of the number of basis functions, and in real calculations becomes excessively large. Therefore, to make the algorithm accomplishable, it is reasonable to limit the number of eigenstates \( \varphi_i \) to a certain number \( N \) of low-lying states making the most contribution to Monte Carlo statistics.

In the next section, the described scheme is implemented and applied for studying of Hubbard-like models of interacting fermions.

### 3. Results

The Hamiltonian of the Hubbard model has the following form:

\[
H = -t \sum_{(ij)\sigma} (c^+_{i\sigma} c_{j\sigma} + c^+_{j\sigma} c_{i\sigma}) - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_{i\sigma} n_{i\sigma} (n_{i\sigma} - 1),
\]  

(8)

where operator \( c_{i\sigma}^+ \) creates an electron with spin \( \sigma \) on site \( i \); \( n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma} \); \( t \) is the amplitude of electron hopping between nearest neighbor sites; \( U \) is on-site Coulomb interaction and \( \mu \) is the chemical potential.

We consider the simplest case when the Hamiltonian (8) is defined on one-dimensional lattice. Then, the cluster will be a chain of \( L_c \) sites, and

\[
H_{\text{inter}} = -t \sum_{\alpha\sigma} \left( c_{1,\alpha\sigma}^+ c_{L_c,(\alpha-1)\sigma} + c_{L_c,(\alpha-1)\sigma}^+ c_{1,\alpha\sigma} \right),
\]  

(9)

where \( \alpha = 1, \ldots, N_c \) and periodic boundary conditions are assumed. The more is the length of the chain \( L_c \), the more accurate the decomposition (5) will reproduce the true eigenfunction of the whole system. On the other hand, the number of relevant low-energy levels of the cluster should be big enough to capture the physics of the model.

Figure 3 shows the low-energy level structure for a chain of \( L_c = 6 \) sites; the parameters of the Hamiltonian (8) are \( U = 4, \mu = -2 \) (in units of \( t \)); this value of \( \mu \) corresponds to the half-filling.
Figure 3. Level structure for cluster of 6 sites. $U = 4; \mu = -2$. Levels corresponding to the half-filling are shown in black.

The total number of states for this cluster is $R = 4096$; the lowest hundred levels are shown in figure 3; most of them are degenerate. As CTWL algorithm works in grand canonical ensemble, the levels can be grouped by the number of particles in the corresponding eigenstates. At fixed $\mu = U/2$, relative positions of levels corresponding to half-filling and deviation from half-filling depend strongly on the ratio $U/t$. For CTWL scheme, it is important to have a good variety of basis functions from various sectors of particle numbers, since in this case update processes are performed more efficiently. Horizontal green lines show possible truncations of high-lying states and corresponding numbers of low-lying states which are kept.

During Monte Carlo process, the system evolves in the phase space $R^d \otimes \tau$ of $d$ space coordinates and imaginary time $\tau \in [0; \beta]$, $\beta = 1/T$ is the inverse temperature. The probability of realization of a state $i$ of energy $E_i$ is weighted with Gibbs exponent $e^{-\beta E_i}$, and the system spends most of the time in configurations making the most contribution to the partition function. In its initial formulation, the algorithm is ergodic, i.e. there is a nonzero probability of transition from any initial configuration to any final one in the phase space. However, when truncating is applied, some states may become inaccessible. Figure 4 shows the average time spent by the system in low-energy eigenstates for different truncating values; the energy values of the corresponding eigenstates are shown in red. The level structure in figure 3 is such that for $N = 28$ (Fig. 4b) the system is non-ergodic: the probability of realization of states $20 \div 24$ is zero.

As most of Monte Carlo schemes, CTWL algorithm suffers from critical slowing down when decreasing temperature [14], as well as from the sign problem [15]. The last issue is $NP$-hard and greatly suppresses the ability of Monte Carlo algorithms to simulate many-body fermion systems. The presented realization of the algorithm is not an exception. Figure 5 shows the dependence of the energy of the system under study as a function of temperature and the number of low-energy levels $N$ being kept compared with the results obtained by simulation in occupation numbers representation.
Figure 4. The histograms of the time spent by the system in various eigenstates during the operation of the CTWL algorithm. $\beta = 1; L_c = 6; N_c = 4; N = 12$ (a); $N = 28$ (b); $N = 61$ (c); $N = 64$ (d).

Figure 5. The results obtained with CTWL algorithm in eigen basis (diamonds) compared with the exact values obtained with CTWL algorithm in occupation numbers representation (solid lines) for various values of truncating $N$. The sign problem becomes a significant obstacle to the convergence of the algorithm with decreasing temperature.

As can be seen, temperature $\beta = 1$ is too high to achieve a reasonable agreement with the exact result, and more levels must be accounted for better matching. The situation is better for $\beta = 2$; however, for greater values of $\beta$ the convergence time increases dramatically, and we were unable to obtain acceptable results for $N > 50$. In this sense, the eigen basis functions (5) seem to be less applicable for Hubbard Hamiltonian (8). Nevertheless, we believe that having the presented algorithm at hand and choosing the appropriate representation, one will be able to reduce the sign problem and go down the temperature in calculations. From the practical point of view, the most promising area of application is quasi-one-dimensional multi-orbital models with complex multi-particle interactions.
4. Conclusions
We have developed new generalized continuous-time quantum Monte Carlo algorithm which is absolutely universal in the sense that it allows to calculate models specified in an arbitrary basis (in the basis of occupation numbers; in the momentum representation; in the basis of the eigenfunctions of small clusters into which the entire system is divided, or in any other basis): only the specification of the matrix elements between the basis functions defined in a convenient basis is needed. The implemented algorithm was applied to one-dimensional Hubbard model.

The algorithm will be especially useful in studying complex multi-orbital low-dimensional models.

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