Complex diffusion Monte-Carlo method: test by the simulation of the 2D fermions

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COMPLEX DIFFUSION MONTE-CARLO METHOD: TEST BY THE SIMULATION OF THE 2D FERMIONS

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Abstract

On the base of the diffusion Monte-Carlo method we develop the method allowing to simulate the quantum systems with complex wave function. The method is exact and there are no approximations on the simulations of the module and the phase of the system’s wave function. In our method averaged value of any quantity have no direct contribution from the phase of distribution function but only from the phase of the Green function of diffusion equation. We test the method by the simulations of the ground state of fermions in two-dimensional parabolic well. Anyons are used for the representation of the two-dimensional (2D) fermions. We vary the number of fermions from two to ten and find a good agreement of the numerical results with analytical ones for the numbers of the particles $N > 4$.

Keywords: anyon, Monte-Carlo simulation, fermions, ground state.

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1 Introduction

There are several objects of the quantum mechanics where the investigated system’s wave function is essentially complex (having imaginary part). The examples of these objects are a two-dimensional system of electrons in the external uniform magnetic field when vector potential has a central-symmetric form and system of anyons. The complexity of wave function does not give a possibility for the simulations of such kind of systems by using well-known Green Function Monte-Carlo method (see review [1]). This method essentially demand the reality of the system’s wave function which considered as probability weight in during stochastic process.

There had been undertaken the several attempts [2, 3, 4] for the construction a method for the simulation of quantum systems with complex wave function. Authors
of the works [2, 6] suggested to take as a probability weight the module of the complex distribution function. All quantities are calculated in [2, 6] by averaging over this complex distribution function. The phase of this function $\gamma$ is taken accordingly $\gamma = \sum \gamma_i$, where $\gamma_i$ is the phase at the $i$-time step of the stochastic process.

Another quantum Monte Carlo method using algorithm without branching for the simulating of complex problems was developed in [4]. The main trouble of this approach was an increasing of the statistical error as a function of the whole time of the simulation.

In the previous paper [5] it was suggested new Complex Diffusion Monte-Carlo (CDMC) method allowing to simulate the quantum systems with complex wave function. Our method is rather close to the fixed - phase Diffusion Monte-Carlo method developed for the simulation of the two-dimensional electrons in the magnetic field [3]. In this work there had been an exact simulation only of the module of system’s wave function. The phase of the wave function was considered as fixed and equal to phase of the Laughlin’s wave function [7]. In contrast, our method include also the simulation of the phase factor of the wave function.

The basic difficulty of the numerical simulation of the fermions is essentially the same as for the systems with the complex wave function. Their wave function can change the sign and therefore can not be used as the probability weight in the simulation process.

For the simulation of the continuum (not on the lattice) fermionic systems it were developed widely used fixed node Monte-Carlo method [8]( see also reviews [1, 9]) and recently proposed constrained path Monte-Carlo method [10]. In these both methods it was assumed the restriction on the random walks connected with the uncertainties in the space localization of the wave function node surfaces. The comparison of these methods was done in [11].

In the $2D$ space we have unique tool – so-called anyons, particles (bosons or fermions) with additional gauge interaction which provide needed statistical properties [12, 13]. So, by tuning the coupling constant we may arrive to the fermions starting from the bosons. It looks very attractive to apply the anyons for the simulation of the $2D$ fermions, because statistical vector potential that gives anyonic property is relatively smooth and continuous [13, 14]. The remaining main problem is that the wave function of anyonic system is essentially complex, i.e. it contains an imaginary part.

The CDMC method was successfully tested by the simulation of ground state of
one electron in magnetic field [5]. In the present work we briefly outline the idea of CDMC (the details of the algorithm one can find in [5]) and provide a further test it by simulating the ground state of fermions in 2D parabolic well and comparing with well known analytical answer for the ground state energy as a function of the number of fermions. The simulation is done for the fermionic systems with the number of particles from two to ten. It was found a good agreement of the numerical results with analytical ones for the numbers of the particles great than four. This observation of the fermionic simulation allows us to hope that the CDMC is a good tool for the simulation of 2D fermion systems.

2 Model and CDMC method for the simulation

Hamiltonian of anyons in the 2D parabolic well has a form:

\[ \hat{H} = \frac{1}{2M} \sum_{i=1}^{N} \left( \vec{p}_i + \vec{A}(\vec{r}_i) \right)^2 + \frac{M}{2} \sum_{i=1}^{N} \vec{r}_i^2. \]  

(1)

Here \( M \) is the mass of particle, \( \vec{p} = -i\hbar \vec{\nabla} \), where \( \vec{\nabla} = \vec{i} \frac{\partial}{\partial x} + \vec{j} \frac{\partial}{\partial y} \), \( \omega_o \) stands for characteristic frequency of free particles in 2D parabolic well and \( \vec{r}_i \) is radius vector of \( i \)-th particle. The number of particles is \( N \).

Vector potential for anyons \( \vec{A}(\vec{r}_i) \) [13, 14] in (1) is

\[ \vec{A}(\vec{r}_i) = \hbar \nu \sum_{j>i} \frac{\vec{z} \times \vec{r}_{ij}}{|\vec{r}_{ij}|^2}. \]  

(2)

Here \( \vec{z} \) is unit vector perpendicular to 2D plane and \( \nu \) characterizes the form of fractional statistics (spin of the anyon). In this work we want to employ a bosonic representation of anyons, therefore \( \nu = 0 \) corresponds to noninteracting bosons and \( \nu = 1 \) is the case of our interest – free fermions.

In CDMC a Monte Carlo simulation is carried out with the complex distribution function

\[ f(\vec{R}, t) = \Psi_T^*(\vec{R})\Psi(\vec{R}, t), \]  

(3)

where \( \vec{R} \) stands for the coordinates of all particles, \( \Psi_T(\vec{R}) \) is a trial wave function and the wave function \( \Psi(\vec{R}, t) \) satisfies a Schrödinger equation with imaginary time (expressed in \( \hbar \) units)

\[ -\frac{\partial \Psi(\vec{R}, t)}{\partial t} = (\hat{H} - E_T)\Psi(\vec{R}, t). \]  

(4)
With a suitable choice of a trial energy $E_T$ it is possible to arrange the convergence
$\Psi(\vec{R}, t) \rightarrow \Psi_0(\vec{R})$ – an exact stationary wave function of ground state of Hamiltonian
(1) at $t \rightarrow \infty$ [8].

For a bosonic representation of anyons we take (conjugated) trial wave function
in the form:

$$\Psi^*_T(\vec{R}) = \prod_{i=1}^N \Psi^*_T(\vec{r}_i).$$

(5)

Good choice of single particle trial wave function $\Psi^*_T(\vec{r}_i)$ (see below) as energy $E_T$
must provide a convergence of simulation process to exact ground state.

The distribution function $f \equiv f(\vec{R}, t)$ satisfies a diffusion equation:

$$-\frac{\partial f}{\partial t} = -D \sum_{i=1}^N \Delta_i f + \sum_{i=1}^N \nabla_i(f \text{Re} \tilde{F}_Q(\vec{r}_i)) +$$

$$+ i \sum_{i=1}^N [\nabla_i(D \text{Im} \tilde{F}_Q(\vec{r}_i)) - \frac{\hbar}{M} \tilde{A}(\vec{r}_i) \nabla_i f] + (E_L(\vec{R}) - E_T) f.$$

(6)

Here $D = \frac{\hbar^2}{2M}$, $\Delta_i = \nabla_i^2$. When a time step integration of diffusion equation (6), $\tau$, goes to zero, then Green function for this equation has a form:

$$G(\vec{R}, \vec{R}'; \tau) = \frac{\exp[D\tau \sum_{i=1}^N \tilde{A}_Q^2(\vec{r}_i, \vec{r}_i')] / (4\pi D\tau)^N}{\times}$$

$$\times \exp \left[ \sum_{i=1}^N (\vec{r}_i - \vec{r}_i' - D\tau \text{Re} \tilde{F}_Q(\vec{r}_i'))^2 / 4D\tau \right] \times$$

$$\times \exp \left[ i \sum_{i=1}^N \tilde{A}_Q(\vec{r}_i, \vec{r}_i')(\vec{r}_i - \vec{r}_i' - D\tau \text{Re} \tilde{F}_Q(\vec{r}_i')) \right].$$

(7)

In the expressions (6) and (7)

$$\tilde{F}_Q(\vec{r}_i) = 2\Psi^{*-1}_T(\vec{r}_i) \nabla_i \Psi^*_T(\vec{r}_i),$$

(8)

$$E_L(\vec{R}) = \Psi^{*-1}_T(\vec{R}) \hat{H}' \Psi^*_T(\vec{R}),$$

(9)

$$\hat{H}' = \frac{1}{2M} \sum_{i=1}^N (\vec{p}_i - \vec{A}(\vec{r}_i))^2 + \frac{Mw_o^2}{2} \sum_{i=1}^N \vec{r}_i^2.$$

(10)
In general case $\Psi^*_T(\vec{r}_i)$ is a complex wave function and
\[ \vec{F}_Q(\vec{r}_i) = \text{Re}\vec{F}_Q(\vec{r}_i) + i\text{Im}\vec{F}_Q(\vec{r}_i). \] (11)

In (7) (see also [5]) we have introduced a new quantity
\[ \vec{A}_Q(\vec{r}_i, \vec{r}_i') = \frac{1}{2i}\text{Im}\vec{F}_Q(\vec{r}_i') - \frac{1}{\hbar}\vec{A}(\vec{r}_i). \] (12)

In the expressions (7) and (12) vectors $\vec{R}$ and $\vec{r}_i$ correspond to time point $t + \tau$ and vectors $\vec{R}'$, $\vec{r}_i'$ to time point $t$.

One can see that the Green function $G(\vec{R}, \vec{R}'; \tau)$ (7) as and distribution function $f$ in (3) is a complex. These both quantities are satisfying to the usual integral relation
\[ f(\vec{R}, t + \tau) = \int d\vec{R}' G(\vec{R}, \vec{R}'; \tau) f(\vec{R}', t). \] (13)

From relation (13) it is following that the module and phase of the distribution function at consequent time point are determining by the module and the phase of the Green function and of ones of the distribution function at previous time point of integration of diffusion equation (6).

As the energy $E_L(\vec{R})$ is a complex, real and imaginary part of $E_L(\vec{R})$ contribute separately to ones of the Green function. Therefore the expression of the last two exponents in (7) has a form:
\[ \exp \left[ -\tau(\text{Re}E_L(\vec{R}) - E_T) \right] \times \]
\[ \times \exp \left[ i \sum_{i=1}^{N} \vec{A}_Q(\vec{r}_i, \vec{r}_i')(\vec{r}_i - \vec{r}_i' - D\tau\text{Re}\vec{F}_Q(\vec{r}_i')) - i\tau\text{Im}E_L(\vec{R}) \right] . \] (14)

The mean value of the some quantity $B(\vec{R}(t))$ on the complex distribution function $f(\vec{R}, t)$ at the time $t$ of the simulating process is calculated by the formula (see [2, 6])
\[ < B(t) > = \frac{\sum_{i=1}^{M} \exp[i\gamma(\vec{R}_i(t))]B(\vec{R}_i(t))}{\sum_{i=1}^{M} \exp[i\gamma(\vec{R}_i(t))]} . \] (15)

Here $\vec{R}_i(t)$ is the coordinates of all particles from the $i$-th configuration of the $M$ - configurations at time $t$. The coordinates $\vec{R}_i(t)$ of particles in (15) are weighted with probability $|f(\vec{R}_i, t)|$ and the quantity $\gamma(\vec{R}_i(t))$ is a phase of the distribution function $f(\vec{R}_i, t)$. 

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From integral expression (13) it is seen that phase of the distribution function \( \gamma(\vec{R}_i(t + \tau)) \) connected with the phase of the Green function \( \gamma_G(\vec{R}_i(t + \tau), \vec{R}_j(t)) \) and the phase \( \gamma(\vec{R}_j(t)) \) of the distribution function by the relation:

\[
\gamma(\vec{R}_i(t + \tau)) = \gamma_G(\vec{R}_i(t + \tau), \vec{R}_j(t)) + \gamma(\vec{R}_j(t)).
\]

Here \( \vec{R}_j(t) \) is \( j \)-th configuration at time \( t \). So, we can write

\[
< B(t + \tau) > = \frac{\sum_{i=1}^{M} e^{i\gamma_G(\vec{R}_i(t+\tau),\vec{R}_j(t)) + i\gamma(\vec{R}_j(t))} B(\vec{R}_i(t + \tau))}{\sum_{i=1}^{M} e^{i\gamma_G(\vec{R}_i(t+\tau),\vec{R}_j(t)) + i\gamma(\vec{R}_j(t))}} = \frac{\sum_{i=1}^{M} e^{i\gamma_G(\vec{R}_i(t+\tau),\vec{R}_j(t))} B(\vec{R}_i(t + \tau))}{\sum_{i=1}^{M} e^{i\gamma_G(\vec{R}_i(t+\tau),\vec{R}_j(t))}}.
\]

(16)

The expression (16) is hold, because all quantities in numerator and denominator are weighted with probability \( |f(\vec{R}_i(t+\tau), t + \tau)| \), i.e. at time moment \( t + \tau \) with new configurations \( \vec{R}_i(t + \tau) \). Hence, a mean quantity \( < B(t + \tau) > \) is determined only by phase \( \gamma_G \) of the Green function. It is a key conclusion, providing the calculation of mean quantities in our CDMC.

Next, by taking into account the expression for the simulation of the random displacement for the particle \( \vec{r}_i = \vec{r}_i + D\tau \text{Re} \vec{F}_Q(\vec{r}_i) + 2(D\tau)^{1/2} \chi \) (see [8] and [5]), where \( \chi \) is a gaussian random number, the expressions for \( \vec{F}_Q(\vec{r}_i) \) (8), for \( E_L(\vec{R}) \) (9) and for \( \vec{A}_Q(\vec{r}_i, \vec{r}_i') \) (12) and also the expression (14), one can show that at \( \tau \rightarrow 0 \) the phase of the Green function \( \gamma_G \) tends to zero as \( \tau^{1/2} \). This property of \( \gamma_G \) together with the formula (16) allows CDMC successfully simulate all mean quantities.

The simulation process starts with mean field approximation of Fetter, Hanna and Laughlin [15]. In this approximation the mean field \( \overline{\vec{A}} \) generated by the average density \( \rho \) of the particles:

\[
\overline{\vec{A}}(\vec{r}) = \rho \pi \hbar \nu(\vec{z} \times \vec{r}) = \frac{1}{2} \vec{B} \times \vec{r}.
\]

(17)

Here \( \vec{B} = 2\pi \rho \hbar \nu \vec{z} \) is fictitious uniform mean magnetic field that defines corresponding magnetic length \( a_H = \sqrt{\hbar/\rho} \) and cyclotron frequency \( \omega_c = B/M \). Particles move in this mean magnetic field. Energy spectrum of Hamiltonian (1) with \( \overline{\vec{A}} \) and without \( 2D \)
parabolic well is Landau levels. We have to simulate anyonic ground state. Therefore we take a wave function \( \Psi_T^*(\vec{r}_i) \) in the following form:

\[
\Psi_T^*(\vec{r}_i) = C \exp \left( -\alpha \frac{(x_i^2 + y_i^2)}{2R_o^2} \right) \exp \left( -\frac{(x_i^2 + y_i^2)}{4a_H^2} \right).
\]

(18)

Here \( C \) is a normalization constant, \( \alpha \) is numerical parameter and \( R_o = (\hbar/Mw_o)^{1/2} \). In this expression first exponential function with \( \alpha = 1 \) corresponds to the ground state wave function of particle in 2D parabolic well and second one to the ground state of Landau levels.

Average density of particles \( \rho \) is given by \( \rho = 1/\pi r_o^2 \) where \( r_o \) is the mean distance between particles in system. We assume that \( r_o \) equals to \( R_o \). The reason of this is that the interaction between two anyons at any non-zero \( \nu \) has repulsive character and the area \( S_n \) that occupied by free particle at \( n \)-th 2D oscillator’s level is \( S_n = n\pi R_o^2 \). Last relation for \( S_n \) follows by using virial theorem for the quantum energetic states for the free particle in 2D parabolic well.

By substituting expression \( B \) into expression \( a_H \) and taking account that \( \rho = 1/\pi r_o^2 \), we find the following relation between \( a_H \) and \( r_o \): \( a_H = \sqrt{1/2\nu r_o} \). By similar way one can show that \( \hbar \omega_c / 2 = \nu \hbar \omega_o \).

It is natural to use \( \hbar \omega_c / 2 \) as energy unit, \( a_H \) as length unit and \( 2/\hbar \omega_c \) as time unit \( \tau \). In these units the last term of the Hamiltonian (1) has a coefficient \( 1/4\nu^2 \) and the argument of the first exponential function in (18) has a coefficient \( \alpha/4\nu \). By using above relations between \( \hbar \omega_c / 2 \) and \( \hbar \omega_o \) and between \( a_H \) and \( r_o \) it is easily to express the energies in terms of 2D oscillator quanta \( \hbar \omega_o \) and the lengths in terms of \( r_o \).

3 Discussion of the results

The simulation of the ground state of the systems of several fermions in 2D parabolic well was performed. By setting the coupling \( \nu = 1 \) in (2) we get fermions from anyons. This value of \( \nu \) is fixed below. As in [8], the total simulation time \( t \) is divided into several (in our case we took 40) time blocks \( \Delta t \). In every time block \( \Delta t \) initial number of configurations \( N_c \) is chosen equal to 1000 and number of time steps \( \tau \) equal to 30.

We simulate the energy \( E_{SIM} \), mean radius \( \bar{r} \) and mean square of radius of \( \bar{r}^2 \) of the fermionic systems. The calculation of these quantities are performed by the formula (16). Here we take into account that the energy \( E_L(\vec{R}) \) has as a real part \( \text{Re}E_L(\vec{R}) \), and also an imaginary part \( \text{Im}E_L(\vec{R}) \). The number of fermions is varied from two to ten.
The \( \tau \) dependence of the energy \( E_{SIM} \) has a general structure \( A_0 + A_1 \tau^{1/2} \) [8] where \( A_0 \) and \( A_1 \) are the numerical constants.

We have obtained that at a very small \( \tau \) the mean deviation of \( E_{SIM} \) larger than the fluctuations of \( E_{SIM} \). At large \( \tau \) further increasing of it leads to the increasing of the fluctuation of \( E_{SIM} \) and thus to the growing of the population number \( N_p \) (the population number \( N_p \) is connected with first exponential function in (14) and was also introduced in [8]). The very large values of \( \tau \) give a dramatical increasing of \( N_p \) that leads to the instability of \( E_{SIM} \) and whole stochastic process. So, we have to choose optimal time step \( \tau_0 \).

CDMC [5] has an artifact that the averaged real quantities become complex, but real parts of them are essentially bigger than imaginary parts because the imaginary parts are controlled by the phase of the Green function \( \gamma_G \) depending as \( \tau_0^{0.5} \). Then the imaginary part of \( E_{SIM} \) for almost all number of fermions \( N \) is less than 0.15 percent of its real part. For \( \overline{\tau} \) and \( \overline{r^2} \) they are less than 0.07 percent of their real parts. 

Table 1 present the exact analytical result for the ground state energy of the fermionic systems in the 2D parabolic well \( E_{EXACT} \), \( E_{SIM} \) (in \( \hbar \omega_o \) units) and the simulated values of \( \overline{\tau} \) and \( \overline{r^2} \) ( in \( r_o \) and \( r_o^2 \) units respectively). The values of \( E_{EXACT} \) was calculated by occupying the available lowest states. The energy of \( K \)-th quantum number state of the 2D oscillator is \( E_K = \hbar \omega_o(K + 1) \) and degeneracy number of this state is equal \((K + 1)\) [16].

\( E_{SIM} \) is depended on value of numerical parameter \( \alpha \) in the trial wave function \( \Psi_T(\vec{r}_i) \) (18). We take \( \alpha \) providing minimal value of the energy \( E_{SIM} \). The numerical data of \( \alpha \) that give a minimal energy \( E_{SIM} \) are outlined also in the Table 1. We have compared the CDMC dependence of the parameter \( \alpha \) versus number of particles \( N \) with the variational calculation of \( \alpha \) [17]. If at the changing of \( N \) from two to ten CDMC \( \alpha \) changes from -0.593 to -0.084, so variational \( \alpha \) changes from -0.293 to -0.683 (see [17]). For the big number fermions (as one can see from table) CDMC \( \alpha \) is almost the same for all systems. Thus a mean field approximation of Fetter, Hanna and Laghlin [15] with numerical parameter in a wave function can be considered as a good start approximation for the simulation of a big number anyons. Table 1 also shows the numerical values of the population number \( N_p \) and optimal time steps \( \tau_0 \). Good agreement of the simulation results for the \( E_{SIM} \) with the exact ground state energies \( E_{EXACT} \) for the numbers of the particles bigger than four allows us to hope that CDMC [5] gives a possibility for the exact simulation of the big number 2D fermions.
Table 1: The energies of the fermion systems in 2D parabolic well. Here $N$ – numbers of particles, $E_{EXACT}$ – analytically calculated ground state energies (in $\hbar \omega_o$ units), $E_{SIM}$ – results of the simulation ground state energies (in $\hbar \omega_o$ units), $\bar{r}$ – the numerical values for the simulated mean radius (in $r_o$ units), $\bar{r}^2$ – the numerical values for the simulated mean square radius (in $r_o^2$ units), $\alpha$ – the numerical parameters in the trial wave function (18) that gives a minimum $E_{SIM}$, $N_p$ – the population numbers and $\tau_0$ – the optimal time steps. All simulated quantities and their deviations from mean values were averaged over 30 last time blocks $\Delta t$ when $E_{SIM}$ and $N_p$ have had relatively stable values.

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<th>$E_{SIM}$</th>
<th>$\bar{r}$</th>
<th>$\bar{r}^2$</th>
<th>$\alpha$</th>
<th>$N_p$</th>
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<td>0.01</td>
</tr>
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<td></td>
<td></td>
<td>±9.595·10^{-2}</td>
<td>±1.061·10^{-2}</td>
<td>±6.435·10^{-2}</td>
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<tr>
<td>10</td>
<td>30</td>
<td>30.905</td>
<td>2.601</td>
<td>8.599</td>
<td>-0.084</td>
<td>1032 ± 23</td>
<td>0.005</td>
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<td>±2.010·10^{-1}</td>
<td>±2.839·10^{-2}</td>
<td>±2.095·10^{-1}</td>
<td></td>
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<td></td>
</tr>
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</table>
References


[17] Abdullaev B., Musakhanov M. and Nakamura A. Approximate formula for the ground state energy of anyons in $2D$ parabolic well. cond-mat/0012423, pp. 7 (2000).