Limits of the Quantum Monte Carlo method

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Abstract

We consider the one-dimensional quantum-statistical problem of interacting spin-less particles in an infinite deep potential valley and on a ring. Several limits for the applicability of the quantum Monte Carlo methods were revealed and discussed. We show the inapplicability of the quantum Monte Carlo method for ring-like geometries, realize an unphysical frustration for interacting fermions and a minus-sign problem for interacting bosons.

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I. INTRODUCTION

Quantum Monte Carlo (QMC) methods are known to be powerful tools in studying various quantum-statistical problems like quantum-spin models, Hubbard or t-J models, quantum chromodynamical systems or interacting fermions in real space. It is believed that the method has great potentials to handle analytically difficult and complex problems. The main idea of the method is to transform a $d$ dimensional quantum-statistical problem in $d+1$ dimensional classical one, by a procedure closely related to the Path integral formalism of quantum mechanics. Due to the increased dimensionality the method is computer-time consuming. Nowadays, the accessible and powerful modern computers makes the method more and more popular.

As an exercise for the applicability of QMC methods we studied the quantum-statistical problem of several short-range interacting quantum particles in one-dimensional space. During this exercise we found however several technical and conceptual difficulties which limits the applicability of the method. The present paper intends to discuss the problem in this sense.
II. THE METHOD

In this section we review briefly the method of studying short-range interacting quantum particles in real 1D spaces by the QMC method. We will neglect the spin variables and consider idealized spin-less fermions or bosons.

The time-independent Schrödinger equation for a single particle with mass $m$ in 1D is:

$$\hat{H}\psi = -\frac{\hbar^2}{8\pi^2 m}\Delta\psi + V(x) = E\psi. \quad (1)$$

Discretizing the problem on a lattice with sites of length $a$, the differential equation (1) can be written in the form of $L (aL = l$ with $l$ the length of the considered space) coupled linear equations

$$\left(-\frac{\hbar^2}{8\pi^2 ma^2}\right)(\psi_{i+1} + \psi_{i-1} - 2 \cdot \psi_i) + V_i \cdot \psi_i = E\psi_i, \quad (2)$$

where $\psi_i$ and $V_i$ denotes the medium values in box $i$ of the lattice for the functions $\psi(x)$ and $V(x)$ respectively. Introducing the notations

$$t = \frac{\hbar^2}{8\pi^2 ma^2} \quad (3)$$

$$W_i = V_i + \frac{\hbar^2}{4\pi^2 ma^2}, \quad (4)$$

equation (2) becomes:

$$-t \cdot (\psi_{i+1} + \psi_{i-1}) + W_i \psi_i = E\psi_i \quad (5)$$

We can write now this system of equations in a second quantized form, using as state vectors the $n_i$ occupation number of the cells: $|n_1, n_2, ..., n_i, ..., n_L>$. We consider the $\hat{c}_i^+$ creation, $\hat{c}_i$ annihilation and $\hat{n}_i = \hat{c}_i^+ \hat{c}_i$ occupation number operators defined for bosons as

$$\hat{c}_i^+ | n_1, n_2, ..., n_i, ..., n_L > = \sqrt{n_i + 1} | n_1, n_2, ..., n_i + 1, ..., n_L > \quad (6)$$

$$\hat{c}_i | n_1, n_2, ..., n_i, ..., n_L > = \sqrt{n_i} | n_1, n_2, ..., n_i - 1, ..., n_L > \quad (7)$$

and for fermions ($n_i = \{0, 1\}$) as

$$\hat{c}_i^+ | n_1, n_2, ..., n_i, ..., n_L > = (-1)^{s_i} | 1 - n_i > | n_1, n_2, ..., n_i + 1, ..., n_L > \quad (8)$$

$$\hat{c}_i | n_1, n_2, ..., n_i, ..., n_L > = (-1)^{s_i} n_i | n_1, n_2, ..., n_i - 1, ..., n_L >, \quad (9)$$

where $s_i = \sum_{j=1}^{i-1} n_j$. The wave function of the system becomes

$$\psi = \sum_{i=1}^{L} \psi_i \hat{c}_i^+ | 0, 0, ..., 0 >, \quad (10)$$

and equations (5) can be written as:

$$\sum_{i=1}^{L} [-t(\hat{c}_{i+1}^+ \psi_i + \hat{c}_i^+ \psi_{i+1}) + W_i \hat{c}_i^+ \psi_i] | 0, 0, ..., 0 > = \sum_{i=1}^{L} E\psi_i \hat{c}_i^+ | 0, 0, ..., 0 >. \quad (11)$$
The second quantized form of the Hamiltonian in the discretized space will be:

\[ \hat{H} = -t \sum_i [\hat{c}_i^+ \hat{c}_{i+1} + \hat{c}_{i+1}^+ \hat{c}_i] + \sum_i W_i \hat{n}_i. \]  

(12)

Considering more than one non-interactive particles in the same lattice the Hamiltonian is unchanged. Interactions between the particles will be introduced via extra terms like

\[ \hat{H}_o = V_o \cdot \sum_i \hat{n}_i (\hat{n}_i - 1), \]  

(13)

or:

\[ \hat{H}_1 = V_1 \cdot \sum_i \hat{n}_i \hat{n}_{i+1}. \]  

(14)

Term (13) represent an on-site repulsion, and (14) the interaction between particles in neighboring cells. Depending on the sign of \( V_1 \) this interaction can be attractive or repulsive.

The partition function is given by

\[ Z = Tr(\exp (-\beta \cdot \hat{H})) = \sum_{\{n_i\}} \langle n_1, n_2, ..., n_L | \exp (-\beta \cdot \hat{H}) | n_1, n_2, ..., n_L \rangle, \]  

(15)

where the sum is over all the possible combination of the \( n_i \) occupation numbers subject to the \( \sum_{i=1}^L n_i = N \) (\( N \) the total number of particles) restriction and \( \beta = 1/k_B T \).

For a practically successful realization of the MC simulation we have to rewrite the \( Z \) partition function in a form in which calculation of the \( P \) transition probabilities are easy when only a few \( n_i \) occupation numbers have been changed. We will sketch how is possible this.

Denoting by \( V_i \) the interaction terms of the forms \( V_o \hat{n}_i (\hat{n}_i - 1) \) and, \( V_1 \hat{n}_i \hat{n}_{i+1} \), we separate our Hamiltonian in two commuting parts \( \hat{H}_a \) and \( \hat{H}_b \).

\[ \hat{H}_a = (-t \hat{c}_1^+ \hat{c}_2 - t \hat{c}_2^+ \hat{c}_1 + \frac{V_1}{2} + \frac{V_2}{2}) + \]

\[ (+(-t \hat{c}_3^+ \hat{c}_4 - t \hat{c}_4^+ \hat{c}_3 + \frac{V_3}{2} + \frac{V_4}{2}) + ....) \]

\[ + (-t \hat{c}_{L-1}^+ \hat{c}_L - t \hat{c}_L^+ \hat{c}_{L-1} + \frac{V_{L-1}}{2} + \frac{V_L}{2}) = \]

\[ = \hat{H}_1 + \hat{H}_3 + ... + \hat{H}_{L-1}, \]  

(16)

with:

\[ \hat{H}_i = -t \hat{c}_i^+ \hat{c}_{i+1} - t \hat{c}_{i+1}^+ \hat{c}_i + \frac{V_i}{2} + \frac{V_{i+1}}{2}. \]  

(17)

In a similar way \( \hat{H}_b = \hat{H}_2 + \hat{H}_4 + .... + \hat{H}_L \). One will observe immediately that the terms inside \( \hat{H}_a \) and \( \hat{H}_b \) commute, and so:

\[ \langle n_i \rangle | \exp (-\beta \hat{H}_a) | n_j \rangle = \langle n_i \rangle | \exp (-\beta \hat{H}_1) | n_j \rangle \cdot \]

\[ \cdot \langle n_i \rangle | \exp (-\beta \hat{H}_3) | n_j \rangle \cdot .... \cdot \langle n_i \rangle | \hat{H}_{L-1} | n_j \rangle. \]  

(18)
The same equation is valid for $\hat{H}_b$.

Ideal it would be to write the partition function as product of exponentials, each of them containing one $\hat{H}_i$ term. In this way the calculation of the transition probabilities when only a few occupation numbers are changed would be easier. To achieve this we need to write $\exp[-\beta(\hat{H}_a + \hat{H}_b)]$ as: $\exp(-\beta \hat{H}_a) \cdot \exp(-\beta \hat{H}_b)$. Unfortunately this equation is not valid anymore, because $\hat{H}_a$ and $\hat{H}_b$ do not commute.

However, for two $\hat{A}$ and $\hat{B}$ sufficiently small operators one can use the approximation:

$$e^{\hat{A}} \cdot e^{\hat{B}} = e^{\hat{A} + \hat{B} + 0.5 \cdot [\hat{A}, \hat{B}]} \approx e^{\hat{A} + \hat{B}}. \quad (19)$$

Considering now $M$ a large integer, so that $\frac{\beta \hat{H}_a}{M}$ and $\frac{\beta \hat{H}_b}{M}$ is small enough, we are able to use the (19) approximation in the form proposed by Trotter and Suzuki [7]:

$$Z = \sum_{\{n_i\}} <\{n_i\}| (\exp[-\frac{\beta}{M} \cdot (\hat{H}_a + \hat{H}_b)])^M | \{n_i\} > \approx \sum_{\{n_i\}} <\{n_i\}| (\exp[-\frac{\beta}{M} \cdot \hat{H}_a] \cdot \exp[-\frac{\beta}{M} \cdot \hat{H}_b])^M | \{n_i\}> \quad (20)$$

In order to write $Z$ as a product, which in a MC simulation can be considered as transition probabilities, we insert between each exponentials in (20) a complete set of states:

$$\sum_{\{n_{i,j}\}} | n_{1,j}, n_{2,j}, ..., n_{L,j} > < n_{1,j}, n_{2,j}, ..., n_{L,j} |. \quad (21)$$

Because each of these $2M-1$ sets represent an independent sum over all possible states, they will be indexed with a new label, $j$, different from the spatial one, $i$. The initial trace contribute also to the independent set of states, so the $j$ index can take $2M$ values. Remembering that $\hat{H}_i$ acts only on the states $n_i$ and $n_{i+1}$ we can write:

$$Z \approx \sum_{\{n_{i,j}\}} 2^M \prod_{j=1}^{L} P_{i,j}. \quad (22)$$

When $j$ and $i$ are both even or odd the $P_{i,j}$ factors are calculable as

$$P_{i,j} = < n_{i,j}, n_{i+1,j} | e^{(-\Delta \tau \cdot \hat{H})} | n_{i,j+1}, n_{i+1,j+1} >, \quad (23)$$

and $P_{i,j} = 1$ for all other choices (we used the notation $\Delta \tau = \frac{\beta}{M}$).

Because both $i$ and the $j$ indices label occupation numbers, by using the Trotter-Suzuki (T-S) approximation we created a two-dimensional lattice from our real one-dimensional one. Every box of the original lattice is multiplied $2M$ times, and all the $n_{i,j}$ sets ($j = 1, 2M$) are independent. Due to the original trace the $j$ index must satisfy the periodical boundary conditions: $n_{i,2M+1} = n_{i,1}$.

We are able now to consider our quantum-statistical problem as a classical one, characterized by the

$$Z \approx \sum_{\{n_{i,j}\}} \exp(-\beta \sum_{i,j} e_{i,j}) \quad (24)$$
partition function. In equation (24) we used the $-\beta e_{i,j} = \ln P_{i,j}$ notation and every $e_{i,j}$ is calculable from the four $n_{i,j}$, $n_{i+1,j}$, $n_{i,j+1}$ and $n_{i+1,j+1}$ occupation numbers.

We have transformed our quantum-statistical problem in a classical one, considered in a space with increased dimensionality. The dimension indexed by $i$ is called spatial, and the one indexed by $j$ the Trotter or imaginary time direction. The presented method is totally equivalent with the Path Integral [6] formulation of the quantum-mechanical problem. (Each two lines in the Trotter direction corresponding to a time interval $\Delta \tau$ in the Path Integral formalism.)

The Monte Carlo simulation will follow now the known Metropolis algorithm. In the transformed, (24) problem we have four-site interactions between the neighboring sites $n_{i,j}$, $n_{i+1,j}$, $n_{i,j+1}$ and $n_{i+1,j+1}$, with the values of $i$ and $j$ both even or odd (otherwise $e_{i,j} = 0$). In the $i$ and $j$ space this interaction can be represented by a check-board pattern (Fig. 1), with interactions around the dark plaquettes.

In many cases the $P_{i,j}$ probabilities (23) are zero, and so the corresponding state is realized with zero probability. The condition for $P_{i,j} \neq 0$, is:

$$n_{i,j} + n_{i+1,j} = n_{i,j+1} + n_{i+1,j+1}. \quad (25)$$

One will realize immediately that in MC simulations the changes leading to acceptable configurations are quite limited. To save precious computer time and calculations, we must know from the beginning which changes will give nonzero transition probabilities. The acceptable changes (leading to nonzero transition probabilities ) will be:

- the occupation numbers from the left side of a white plaquette are increased by unity, and the values from the right side decreased by unity
- the occupation numbers from the left side of a white plaquette are decreased by unity, and the values from the right site increased by unity

(These changes can be done only if the occupation numbers will not become negative, or for fermions if they are not bigger than one.)

It is obvious that by satisfying initially the (25) conditions for the whole system, and by considering only the above mentioned changes in the occupation numbers, the algorithm will lead to configurations keeping (25).

The Metropolis MC algorithm will be now as follows:

- we consider an initial configuration so that condition (25) holds for the whole lattice
- we change the values of the occupation numbers around a white plaquette in the way described earlier
- we calculate the change in the total energy of the system as $\Delta E = \sum \Delta e_{i,j}$, the sum being done on the neighboring dark plaquettes
- we accept this change with a probability

$$P = \frac{\exp (\beta \Delta E)}{\exp (\beta \Delta E) + 1} \quad (26)$$
• we continue the algorithm until thermodynamic equilibrium is approached

• we collect periodically the relevant data.

We define one MC step as \(2ML\) trials of changing the configuration of the system.

III. DETERMINING THE RELEVANT PHYSICAL QUANTITIES

The relevant physical quantities are determined after the equilibrium dynamic is approached, by averaging over many MC steps (usually of order \(10^5\)). The \(E\) average energy and the \(C\) heat-capacity is computed by using the known equations:

\[
E = -\frac{\partial \ln Z}{\partial \beta} \tag{27}
\]

\[
C = \frac{1}{kT^2} \frac{\partial^2 \ln Z}{\partial \beta^2} \tag{28}
\]

Keeping in mind that the \(e_{ij}\) factors are also functions of \(\beta\) from \((24)\) we get:

\[
E = \left\langle \sum_{i,j} e_{ij} \right\rangle + \left\langle \beta \sum_{i,j} \frac{\partial e_{ij}}{\partial \beta} \right\rangle \tag{29}
\]

\[
C = \frac{1}{kT^2} \left( \left\langle \left( \sum_{i,j} e_{ij} + \beta \sum_{i,j} \frac{\partial e_{ij}}{\partial \beta} \right)^2 \right\rangle - \left\langle \sum_{i,j} e_{ij} + \beta \sum_{i,j} \frac{\partial e_{ij}}{\partial \beta} \right\rangle^2 \right) - \frac{1}{kT^2} \left( 2 \sum_{i,j} \frac{\partial e_{ij}}{\partial \beta} + \beta \sum_{i,j} \frac{\partial^2 e_{ij}}{\partial \beta^2} \right) \tag{30}
\]

In the above formula all the sums are over the dark plaquettes of the lattice and the averaging is an ensemble average, which in our QMC scheme is an average over different MC steps.

IV. CALCULATION OF THE \(E_{I,J}\) FACTORS

We will calculate the \(e_{ij}\) "energies" both for one particle and for many interacting fermions and bosons. For the later case we will assume that the interaction potential between the particles in the same cell is two times stronger than the one between two particles in the nearest cells. We will also assume that there is no external potential energy, thus \(W_i = 2t\).

A. One quantum particle

The Hamiltonian of the particle depends on the kinetic energy only:

\[
\hat{H} = -t \sum_{i=1}^{L} (\hat{c}_{i+1}^\dagger \hat{c}_i + \hat{c}_i^\dagger \hat{c}_{i+1}) + 2t \cdot \sum_{i=1}^{L} n_i \tag{31}
\]

We use the symmetric form:
\[
\hat{H}_i = -t \cdot (\hat{c}^{+}_i \hat{c}^+_i + \hat{c}^{+}_i \hat{c}^+_i) + t \cdot \hat{n}_i + t \cdot \hat{n}_{i+1} \quad \text{where } i = 1, L \tag{32}
\]

\[
\hat{H} = \sum_i \hat{H}_i = -t \sum_{i=1}^L \hat{O}_i \tag{33}
\]

\[
\hat{O}_i = (\hat{c}^{+}_i \hat{c}^+_i + \hat{c}^{+}_i \hat{c}^+_i) - \hat{n}_i - \hat{n}_{i+1}, \quad \text{where } i = 1, L. \tag{34}
\]

One can write the \(e_{ij}\) values as:

\[
e_{ij} = -\frac{1}{\beta} \ln \left( \sum_{k=0}^{\infty} \left( \frac{\beta t}{M} \right)^k \cdot \frac{1}{k!} < n_{i,j}, n_{i+1,j} | \hat{O}_i^k | n_{i,j+1}, n_{i+1,j+1} > \right) \tag{35}\]

\(e_{ij}\) depends only on the occupation numbers \(n_{i,j}, n_{i+1,j}, n_{i,j+1}, n_{i+1,j+1}\), thus

\[e_{ij} = e_{ij}(n_{i,j}, n_{i+1,j}, n_{i,j+1}, n_{i+1,j+1}). \]

For one particle

\[
\sum_{i=1}^L n_{i,j} = 1, \tag{36}
\]

and only the terms with \(n_{i,j} + n_{i+1,j} = n_{i,j+1} + n_{i+1,j+1}\) can be different from zero: \(e_{ij}(0,0,0,0), e_{ij}(1,0,1,0), e_{ij}(0,1,0,1), e_{ij}(1,0,0,1)\) and \(e_{ij}(0,1,1,0)\). The \(e_{ij}(0,0,0,0)\) term is zero, and by using the fact that the \(\hat{O}_i\) operators are hermitian it is easy to prove:

\[e_{ij}(1,0,1,0) = e_{ij}(0,1,0,1)\]

\[e_{ij}(1,0,0,1) = e_{ij}(0,1,1,0). \tag{37}\]

Using the immediate

\[
\hat{O}_i|1,0> = 1 \cdot |0,1> - 1 \cdot |1,0> \]

\[
\hat{O}_i|0,1> = 1 \cdot |1,0> - 1 \cdot |0,1>, \tag{38}\]

equations, the two nontrivial \(e_{ij}\) terms can be calculated by a recursion formula:

\[
< 1,0|\hat{O}_i^k|1,0> = < 1,0|\hat{O}_i^{k-1}|0,1> - < 1,0|\hat{O}_i^{k-1}|1,0>
\]

\[
< 1,0|\hat{O}_i^k|0,1> = < 1,0|\hat{O}_i^{k-1}|1,0> - < 1,0|\hat{O}_i^{k-1}|0,1>. \tag{39}\]

Let us denote by \(a_k = < 1,0|\hat{O}_i^k|1,0>\) and \(b_k = < 1,0|\hat{O}_i^k|0,1>\), and rewrite the above recursion:

\[a_k = b_{k-1} - a_{k-1}\]

\[b_k = a_{k-1} - b_{k-1}. \tag{40}\]

Because \(< 1,0|1,0> = 1\) and \(< 1,0|0,1> = 0\) the first terms of these series are \(a_0 = 1\) and \(b_0 = 0\). For \(k > 0\) we get the analytical forms:

\[a_k = (-1)^k \cdot 2^{k-1}\]

\[b_k = (-1)^{k+1} \cdot 2^{k-1}. \tag{41}\]
Substituting these into the expression of the $e_{ij}$ terms (42) we get:

\[ e_{ij}(1, 0, 1, 0) = \frac{1}{\beta} \left( \frac{\beta t}{M} - \ln \left( \cosh \left( \frac{\beta t}{M} \right) \right) \right), \]  
\[ e_{ij}(1, 0, 0, 1) = \frac{1}{\beta} \left( \frac{\beta t}{M} - \ln \left( \sinh \left( \frac{\beta t}{M} \right) \right) \right). \]  

\[ \text{(42)} \]

\[ \text{(43)} \]

**B. Many interacting fermions**

The Hamiltonian in this case is:

\[ \hat{H} = -t \sum_{j=1}^{L} (\hat{c}_{j+1}^+ \hat{c}_{j} + \hat{c}_{j}^+ \hat{c}_{j+1}) + 2t \sum_{j=1}^{L} \hat{c}_{j}^+ \hat{c}_{j} + V_{1} \sum_{j=1}^{L} \hat{n}_{j} \hat{n}_{j+1} \]  
\[ \text{(44)} \]

Let us assume that the particles have charge $q$ and there are rejective forces between them. The interaction is only between the nearest cells, because spin-less fermions can not be simultaneously in the same cell. (This is the manner we impose the antisymmetric wave-function for fermions). The interaction potential is $V_{1}$

\[ V_{1} = \frac{1}{4\pi\varepsilon_{0}} \cdot \frac{q^{2}}{a}, \]  
\[ \text{(45)} \]

where $a$ is the width of the cells.

The Hamiltonian terms are

\[ \hat{H}_{i} = -t (\hat{c}_{i+1}^+ \hat{c}_{i} + \hat{c}_{i}^+ \hat{c}_{i+1} - \hat{n}_{i} - \hat{n}_{i+1} - 2b\hat{n}_{i} \cdot \hat{n}_{i+1}), \]  
\[ \text{(46)} \]

with $b = \frac{V_{1}}{t}$. The occupation numbers for spin-less fermions can be either zero or one, thus $e_{ij}$ has three different values: $e_{ij}(1, 0, 1, 0)$, $e_{ij}(1, 0, 0, 1)$ and $e_{ij}(1, 1, 1, 1)$. The first two were already calculated.

For the calculation of $e_{ij}(1, 1, 1, 1)$ we show that

\[ \hat{O}_{i}^{k}|1, 1 > = -2(1 + b)\hat{O}_{i}^{k-1}|1, 1 >, \]  
\[ \text{(47)} \]

and get:

\[ < 1, 1|\hat{O}_{i}^{k}|1, 1 > = [-2(1 + b)]^{k}. \]  
\[ \text{(48)} \]

Substituting this in the expression of the $e_{ij}$ energy:

\[ e_{ij}(1, 1, 1, 1) = \frac{2t(1 + b)}{M}. \]  
\[ \text{(49)} \]
C. Many interacting bosons

In this case more particles can be in the same cell, so the interaction between particles in the same cell has to be considered too. The Hamiltonian has the following form:

\[
\hat{H} = -t \sum_{j=1}^{L} (\hat{c}_{j+1}^{+}\hat{c}_{j} + \hat{c}_{j}^{+}\hat{c}_{j+1}) + 2t \sum_{j=1}^{L} \hat{c}_{j}^{+}\hat{c}_{j} + V_{1} \sum_{j=1}^{L} \hat{n}_{j}\hat{n}_{j+1} + V_{0} \cdot \sum_{j=1}^{L} \hat{n}_{j}(\hat{n}_{j} - 1). \tag{50}
\]

Let us assume \( V_{0} = 2V_{1} \). In our standard notations:

\[
\hat{H}_{i} = -t(\hat{c}_{i}^{+}\hat{c}_{i+1}^{+} + \hat{c}_{i}^{+}\hat{c}_{i+1} - \hat{n}_{i} - \hat{n}_{i+1} - 2b\hat{n}_{i}\hat{n}_{i+1} - b\hat{n}_{i}(\hat{n}_{i} - 1) - b\hat{n}_{i+1}(\hat{n}_{i+1} - 1)). \tag{51}
\]

In case of \( N \) bosons we have two conditions:

\[
\sum_{i=1}^{L} n_{i,j} = N,
\]

\[
n_{i,j} + n_{i,j+1} = n_{i,j+1} + n_{i+1,j+1}. \tag{52}
\]

Due to the \( i \leftrightarrow i + 1 \) and \( j \leftrightarrow j + 1 \) invariance of the \( e_{ij} \) values we consider only the dark squares with the biggest occupation number in the left bottom corner. For simplicity we introduce the following notation

\[
\langle n_{i,j}, n_{i+1,j} | \hat{O}_{i}^{k} | n_{i,j+1}, n_{i+1,j+1} \rangle = (n_{i,j}, n_{i+1,j}, n_{i,j+1}, n_{i+1,j+1})_{k}, \tag{53}
\]

and calculate the recurrence formula for a given \( n = n_{i,j} + n_{i+1,j} = n_{i,j+1} + n_{i+1,j+1} \) occupation numbers (\( n \in [0, N] \)). If \( n \) is odd and \( n > 1 \):

\[
\left(\frac{n + 2l + 1}{2}, \frac{n - 2l - 1}{2}, \frac{n + 2k + 1}{2}, \frac{n - 2k - 1}{2}\right)_{k} =
\]

\[
\frac{\sqrt{(n + 2k + 3)(n - 2k - 1)}}{4} \left(\frac{n + 2l + 3}{2}, \frac{n - 2l - 3}{2}, \frac{n + 2k + 1}{2}, \frac{n - 2k - 1}{2}\right)_{k-1} +
\]

\[
\frac{\sqrt{(n + 2k + 1)(n - 2k + 1)}}{4} \left(\frac{n + 2l + 1}{2}, \frac{n - 2l - 1}{2}, \frac{n + 2k + 1}{2}, \frac{n - 2k - 1}{2}\right)_{k-1} -
\]

\[
n(1 + b(n - 1)) \left(\frac{n + 2l + 1}{2}, \frac{n - 2l - 1}{2}, \frac{n + 2k + 1}{2}, \frac{n - 2k - 1}{2}\right)_{k}. \tag{54}
\]

The possible values of \( l \) and \( k \) are \( l \in \left[0, \frac{n-1}{2}\right] \) and \( k \in [-l - 1, l] \).
If $n$ is even

\[
\left(\frac{n}{2} + l, \frac{n}{2} - l, \frac{n}{2} + k, \frac{n}{2} - k\right) = \frac{\sqrt{n + 2k + 2n - 2k}}{2}
\left(\frac{n + 2l}{2}, \frac{n - 2l}{2}, \frac{n + 2k + 2}{2}, \frac{n - 2k - 2}{2}\right)_{k-1} + \frac{\sqrt{n + 2k n - 2k + 2}}{2}
\left(\frac{n + 2l}{2}, \frac{n - 2l}{2}, \frac{n + 2k - 2}{2}, \frac{n - 2k + 2}{2}\right)_{k-1} - n(1 + b(n - 1))\left(\frac{n + 2l}{2}, \frac{n - 2l}{2}, \frac{n + 2k}{2}, \frac{n - 2k}{2}\right)_{k},
\]  

(55)

where $l \in \left[0, \frac{n}{2}\right]$ and $k \in [-l, l]$.

This equations carries all the necessary information for calculating numerically the $e_{ij}$ energies.

V. TEST FOR ONE PARTICLE IN AN INFINITE DEEP POTENTIAL VALLEY

We verified our QMC algorithm by considering first one quantum particle (an electron) in an infinite deep potential valley and in contact with a heat-bath at temperature $T$. This simple quantum-statistical problem is easily computable. The energy levels are given by the well-known formula:

\[
E_n = \frac{\hbar^2 n^2}{8mL^2a^2}, \quad (n = 1, 2, \ldots),
\]

(56)

($aL$ is the width of the valley, and was taken $3 \cdot 10^{-9}m$) The expectation value of the energy is numerically computable as:

\[
<E>_t = \frac{\sum_{n=1}^{\infty} E_n e^{\beta E_n}}{\sum_{n=1}^{\infty} e^{\beta E_n}}.
\]

(57)

One can also easily compute theoretically the heat-capacity, of the system by numerically derivating $<E>_t$ as a function of $T$.

Considering a series of simulations with $L = 12$ and $p = \beta t/M = 0.1$ we got the $<E>_t$ values plotted with dots in Fig. 2a. This result is presented in comparison with the $<E>_t(T)$ theoretical curve. On Fig. 2b we plotted together the theoretically computed heat-capacity (dashed line), the one obtained by QMC applying formula (58) (filled circles) and the one obtained from the

\[
C = \frac{\Delta <E>_t}{\Delta T},
\]

(58)

formula (empty circles). The correspondence is satisfactory.
VI. PROBLEM WITH ONE QUANTUM PARTICLE ON A RING

After the promising results for the infinite deep potential valley it is quite frustrating to realize that in this case we cannot solve the original quantum-statistical problem. In the QMC method imposing periodic boundary conditions in the spatial direction will define a problem for a quasi-free particle in constant potential field. The reason for this is that in the QMC formalism we loose the wave-function and remain only with the occupation probabilities. In this manner it is impossible to impose the necessary closing conditions for the wave-function and it’s derivative. From the symmetry of the problem we get only the condition that the occupation numbers have translational invariance. This defines a problem for a free quantum particle (i.e infinite wide potential valley). We expect in this manner to find

\[ <E>_t = \frac{kT}{2}, \]  
\[ C = \frac{k}{2}, \]

(59) \hspace{1cm} (60)

which are the known results for a free particle in contact with a heat-bath at temperature \( T \). In contrast, by imposing the ring-like geometry in the quantum-mechanical problem, the closing condition for the wave-function would yield the

\[ E_n = \frac{\hbar^2 n^2}{2ma^2L^2}, \]  
\( n = 1, 2, 3, \ldots \),

(61)

energy levels and a different \( <E>_t' \) \( (T) \) dependence.

The previous predictions are totally supported by our simulation results. We considered a quantum particle with the mass of an electron, \( aL = 3 \cdot 10^{-9} m \) and \( L = 18 \). On Fig. 3a we plotted the \( <E>_t \) QMC simulation points together with the expected \( <E>_t = kT/2 \) curve (continuous line) and the solution with the discrete \( E_n \) energy levels for the quantum states (dashed line). The simulation results are convincingly supporting the free quantum particle solution. The heat-capacity obtained from formula (30) fluctuates around the expected \( k/2 \) value (Fig. 3b).

Through this simple exercise one can immediately realize a very important limitation for the QMC methods. By loosing the \( \Psi \) wave-function, closing or boundary conditions for \( \Psi \) and it’s derivative are replaced with continuity conditions for \( |\Psi|^2 \) and particle flux \( \vec{j} \). The two problems however are not equivalent, and important differences can be obtained for several problems.

VII. MINUS-SIGN PROBLEM FOR INTERACTING BOSONS

For bosons where the occupation numbers inside one cell can be arbitrary high an immediate difficulty arises when calculating the \( P_{ij} \) transition probabilities. For large occupation numbers the \( P_{ij} \) values become negative, and thus the QMC method is inapplicable. This problem is similar with the well-known minus-sign problem for the Hubbard model [8]. The origin of this non-physical situation is the used Trotter-Suzuki approximation and thus the finite value of \( p = \beta t/M \). As the value of \( p \) is lower more bosons can be considered inside one spatial cell without getting minus sign for \( P_{ij} \). On Fig. 4 as a function
of \( p \) we plotted the maximal boson number per cell for which the \( P_{ij} \) factors are all positive. (We considered here free bosons with the mass and charge of an electron interacting with a repulsive Coulomb potential, and \( a = 1.66 \cdot 10^{-10} m. \)) From this figure we learn that in the limit \( p \to 0 \) the minus-sign problem disappear. Unfortunately in this limit the \( M \) value (lattice size in the imaginary Trotter direction) has to be infinite. The practical solution is of course by fixing the maximal number of bosons in the simulation. This leads to a maximal value of \( p \), and thus a finite \( M \) value. In this manner the minus-sign problem will be eliminated. The technical problem we will face now is that even for small number of bosons the required \( M \) value is large and this limits seriously the applicability of the QMC method for the proposed problem.

**VIII. UNPHYSICAL FRUSTRATION FOR INTERACTING FERMIONS**

In MC-type simulations the usual method for calculating the heat-capacity is by the use of the fluctuation-dissipation theorem. In our case this leads to equation (30), and we get a \( C_1 \) value. An alternative method for calculating the heat-capacity (\( C_2 \)) could be by the definition of this quantity, i.e. by using equation (58).

Considering the problem of interacting fermions (spin-less electrons) on a ring-like geometry we proposed to determine the specific heat of the system both as a function of temperature and particle number in the system. We considered repulsive Coulomb interactions, \( a = 1.66 \cdot 10^{-10} m \), and \( L = 18 \). In order to get confidence in our calculations we used both of the methods. The obtained results were in agreement for low and high fermion number, and totally contradictory for medium occupation density. The logarithm of the ratio (\( C_1/C_2 \)) of the two specific heat is plotted in Fig. 5. Verifying and testing the result in several aspects we got confidence in the obtained differences. The explanation of this strange behavior lies in the space discretization and the way of handling the exclusion principle in QMC simulations. The combined effect of this two introduces a non-physical frustration in the system. This frustration is maximal for half-filled cells and leads to results similar with the ones obtained in spin glasses below the freezing temperature. In MC simulations for spin glasses the difference between the specific heat determined in the two different manner is known [9], and indicates that thermal equilibrium is not completely reached. We encounter a similar situation also here.

To better understand our previous arguments let us follow what is happening in our 2D lattice following the particles paths. Each fermion is represented by a continuous series of 1 values in the Trotter direction which defines the "path" (or the "world-line") of the particle. For fermions these paths cannot intersect each other and can change maximally one cell size for 1 step in the Trotter dimension. A possible path configuration for two fermions is shown as an example in Fig. 6. If we consider more than two fermions, due to the introduced space discretization and the restrictive condition for fermion numbers inside one cell many paths become frustrated. A typical situation for three fermions is shown in Fig. 7. In this setup the path for the fermion in the middle is frustrated in our QMC algorithm. By a no energy change this path can fluctuate between the two neighbors. The energetically stable position is in the middle, but due to our space discretization there is no cell there. We expect that this effect is maximal around the half-filling and disappears for less than three fermions or for complete filling. This prediction is in agreement with the observed results.
The solution for eliminating this unphysical frustration is by considering a fine space discretization where the frustration is minimized. Unfortunately this will increase again the lattice size and create technical problems.

IX. CONCLUSIONS

Considering the quantum statistical problem of interacting particles on a ring-like geometry and in an infinite deep potential valley we realized several limits of the QMC method.

• We loose the concept of wave-function and the method becomes inappropriate for ring-like geometries. Imposing periodic boundary conditions will lead to the problem of particles in a spatially constant potential.

• For interacting bosons we found that due to the considered Trotter-Suzuki transformation a minus-sign problem appears. As the Trotter dimension is increased (the Trotter-Suzuki approximation is improved) more and more bosons per spatial cell can be considered without getting into the minus-sign problem. This problem can be eliminated by increasing the lattice size, which leads to increased computational time.

• For interacting fermions the combined effect of spatial discretization and the application of the exclusion principle creates an unphysical frustration in the system. In this way thermal equilibrium is hard to reach and problems similar to the one obtained in MC methods for spin-glasses are encountered. The effect of this unphysical frustration can be minimized by further increasing the spatial cell numbers, which creates again technical difficulties.

In conclusion, for a successful application of the QMC method on the proposed problem one has to keep in mind and eliminate the above limitations.
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FIGURES

FIG. 1. The characteristic chess-board lattice for the QMC simulations

FIG. 2. QMC results in comparison with the exact theoretical results for an electron in a 1D potential valley with width $aL = 3 \cdot 10^{-9}m$. Fig. 2a presents the energy values of the system as a function of the heat-bath temperature. The dashed curve is theoretical, the filled circles are QMC results. Fig. 2b presents the heat-capacity of the system as a function of the temperature. The dashed curve is the exact theoretical result, filled circles are QMC results obtained by (30), and the empty circles are results obtained from (58). ($L = 12$ and $p = 0.1$)
FIG. 3. QMC results in comparison with theoretical results for an electron on a ring (length of the ring: $3 \cdot 10^{-9} m$). Fig. 3a show the energy values as a function of the heat-bath temperature. Filled circles are QMC simulation results, dashed curve is the desired result for the right quantum-mechanical problem, and the continuous curve presents the theoretical result for a free electron (i.e. infinite large ring). On Fig. 3b we present the heat-capacity of the system as a function of the temperature. Circles are QMC results, obtained by (30), and the line represent the theoretical $k/2$ value for a free particle. ($L = 18$ and $p = 0.2$)

FIG. 4. Maximal bosons number per cell ($n$), for which the minus-sign problem does not appear as a function of the $p$ parameter. We considered bosons with the mass and charge of the electron, interacting with repulsive Coulomb potential. ($a = 1.66 \cdot 10^{-10} m$ and $L = 18$)
FIG. 5. Logarithm of the ratio for the heat-capacity calculated by two different ways ($C_1$ and $C_2$), as a function of particle number per cell. (Interacting fermions with mass and charge of an electron, Coulomb potential, $aL = 3 \cdot 10^{-9} m$ and $L = 18$.)

FIG. 6. A specific path configuration for two fermions

FIG. 7. Example of frustration for three fermions