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Interacting electrons in one dimension: a path integral Monte Carlo study

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Abstract

Path integral Monte Carlo simulations have been carried out for a system of interacting fermionic particles in one dimension. Due to the fact that the sign problem can be completely eliminated for one-dimensional systems, such simulations allow one to obtain accurate energies and particle densities in arbitrary external potentials. Two cases were considered: electrons in the field of a uniform neutralizing background and in an effective field of atoms on a lattice. In the latter case, a clear asymmetry of the charge density distribution of conducting electrons and holes has been observed.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Recent decades have demonstrated an increasing interest to study the properties of strongly correlated electron systems. Understanding of their behaviour is crucially important for further progress in the development of nanoscale microelectronic devices. Also accurate, solely first-principles treatment of interacting electrons is necessary for the description of molecular structure and molecular interactions.

One of the methods which is specially designed for the simulations of systems of interacting quantum particles is the path integral Monte Carlo (PIMC) [1]. This method allows, in principle, us to obtain statistically exact equilibrium averages of physical observables in many-body quantum systems at finite temperatures. A serious difficulty of the PIMC approach in application to electrons is the so-called sign problem. This problem originates in the fact that the wavefunction, describing N fermions (which electrons are), must change sign (be antisymmetric) upon transposition of any two particles. This results in alternating signs in the discretized coordinate representation of the density matrix which defines the weight function

within the PIMC method. At relevant temperatures, contributions from the positive and negative parts of the weight function almost perfectly cancel each other so that there is no hope to extract any useful information.

A remarkable feature of the PIMC approach in one dimension is that the method can be formulated in a way that the sign problem disappears completely. Though this fact was noted already in 1984 [2], and discussed in a more recent review [3], it remained largely unused except perhaps the case of lattice models [4, 5]. It was shown in work [6] that the elimination of the sign problem in one-dimensional case allows one to produce very accurate energies and density distributions for non-interacting fermions in an external field, with the full account for the permutational symmetry. Inclusion of the particle's interactions in the PIMC approach can be done straightforwardly and does not bring any computational difficulties. Thus, the properties of interacting identical fermions in one dimension can also be computed with a high precision.

The aim of this paper is to demonstrate that the PIMC approach is able to provide, from the first principles, very detailed and accurate information on equilibrium properties of strongly interacting electron systems in one dimension. One-dimensional case represents a special interest from both theoretical and experimental points of view. Properties of electron systems in one dimension are usually described in terms of Luttinger liquid [7, 8] with spectral and dynamical properties differing from the Fermi liquid which describes electrons in higher dimensions. From the experimental point of view there is enormous interest to the behaviour of electrons in quantum wires and carbon nanotubes, where motion of electrons is allowed in one dimension but strongly restricted in two others [9–11].

2. Simulated system and methodology

In this work, the PIMC method is applied to compute energies, electron densities and electron correlations in a model of many-electron system in one dimension. At the moment, electrons are considered as spinless (or polarized). They are put in an external potential which in effective way represents a field of atomic nuclei and internal electrons. The adopted functional form of the external potential is

$$V_{\mathrm{ex}}(x) = -\rho_0 \ln(x(L-x)) + A\cos(2\pi m x/L), \tag{1}$$

where x ($0 < x < L$) is the space coordinate and L is the size of the system. The first term of the potential (1) represents the electrostatic potential of a uniform background charge density ρ_0 spread in the interval $[0, L]$. In the examples presented below, the background charge density is approximately equal to the average electron density N/L, so that the whole system is about electroneutral. The second term in (1) creates m equally separated potential wells, which may be considered as effective attraction fields of lattice atoms. Parameter A regulates the strength of the attraction of electrons to these 'atoms'. All quantities are given in dimensionless units with the electron charge, the mass and Planck constant equal to 1. The total potential energy, including electron–electron interactions, is given by

$$V(\{x_i\}) = \frac{1}{2}\sum_{i,j=1;i\neq j}^{N}\frac{1}{|x_i - x_j|} + \sum_{i=1}^{N} V_{\mathrm{ex}}(x_i). \tag{2}$$

The standard path integral Monte Carlo approach is based on the following expansion of the density matrix $\hat{\rho}$ (known also as Trotter expansion) [12]:

$$\hat{\rho} = \exp(-\beta\hat{H}) = \exp\left(-\frac{\beta}{J}\hat{H}\right)\exp\left(-\frac{\beta}{J}\hat{H}\right)\cdots\exp\left(-\frac{\beta}{J}\hat{H}\right) = \prod_{j=1}^{J}\hat{\rho}^{(j)}, \tag{3}$$

where high-temperature (short-time) density matrices $\hat{\rho}^{(j)} = \exp\left(-\frac{\beta}{J}\hat{H}\right)$ are repeated J times. Following the approach of Takahashi [2], each high-temperature density matrix for a fermionic system is presented as sum over permutations of high-temperature density matrices for distinguishable particles, which in the coordinate representation results in

$$\rho^{(j)}\left(x_1^{(j)},\ldots,x_N^{(j)}\middle|x_1^{(j+1)},\ldots,x_N^{(j+1)}\right) = \frac{1}{N!}\left(\frac{J}{2\pi\beta}\right)^{N/2}\sum_P \mathrm{Sign}(P)$$
$$\times\exp\left(-\frac{J}{2\beta}\sum_{i=1}^{N}\left(x_i^{(j)}-x_{P(i)}^{(j+1)}\right)^2-\frac{\beta}{2J}\left(V\left(\left\{x_i^{(j)}\right\}\right)+V\left(\left\{x_{P(i)}^{(j+1)}\right\}\right)\right)$$
$$=\frac{1}{N!}\left(\frac{J}{2\pi\beta}\right)^{N/2}\exp\left(-\frac{\beta}{2J}\left(V\left(\left\{x_i^{(j)}\right\}\right)+V\left(\left\{x_i^{(j+1)}\right\}\right)\right)\right)$$
$$\times\det\begin{vmatrix}\exp\left(-\frac{J}{2\beta}\left(x_1^{(j)}-x_1^{(j+1)}\right)^2\right) & \cdots & \exp\left(-\frac{J}{2\beta}\left(x_1^{(j)}-x_N^{(j+1)}\right)^2\right)\\ \cdots & \cdots & \cdots\\ \exp\left(-\frac{J}{2\beta}\left(x_N^{(j)}-x_1^{(j+1)}\right)^2\right) & \cdots & \exp\left(-\frac{J}{2\beta}\left(x_N^{(j)}-x_N^{(j+1)}\right)^2\right)\end{vmatrix}, \tag{4}$$

where $V\left(\left\{x_i^{(j)}\right\}\right)$ is the total potential energy (2) of all particles at imaginary time (j). The canonical partition function is obtained by substituting (4) into (3) and integrating over all coordinates $\left\{x_i^{(j)}\right\}$

$$Z=\int\prod_{i=1}^{N}\prod_{j=1}^{J}\mathrm{d}x_i^{(j)}\rho^{(j)}\left(x_1^{(j)},\ldots,x_N^{(j)}\,\middle|\,x_1^{(j+1)},\ldots,x_N^{(j+1)}\right) \tag{5}$$

with the boundary conditions $x_i^{(1)} = x_i^{(J+1)}$. By performing Metropolis random walk in the space of $\left\{x_i^{(j)}\right\}$ with the weight function defined by (4), (5), different quantum canonical averages can be calculated [1, 2, 13]. More details of the simulation procedure, concerning the types of the Monte Carlo steps, computations of determinants, etc, are given in the previous paper [6].

3. Results and discussion

A model system consisting of several (9–20) fermionic charged particles in the external potential (1) has been simulated according to the procedure described above. The parameters of different simulation runs are gathered in table 1, as well as computed energies. The background charge density was chosen to be 0.5 which provides the overall neutrality in the reference cases (runs 1, 2, 4) and approximate neutrality in other cases. The reciprocal temperature in all cases was set to $\beta = 50$ which corresponds essentially to the ground state. A number of test simulations with different number of beads $J = 50$–1000 have been performed and value $J = 500$ was chosen for all the production runs as providing convergence relative to further increase of this parameter. The number of MC steps was 10^9 for the equilibration and 5×10^9 for the collection of averages. The production part of each run was divided into ten fragments of 5×10^8 MC steps each, and the statistical uncertainty was evaluated from the variance of intermediate averages computed over these fragments.

Figure 1 shows coordinate density distributions for 10(a) and 20(b) particles, both series of simulations being carried out at the same average particle density (runs 1 and 2 in table 1), in the field of a uniform neutralizing background. The solid lines show charged particles with full exchange interactions. For comparison, the densities of charged

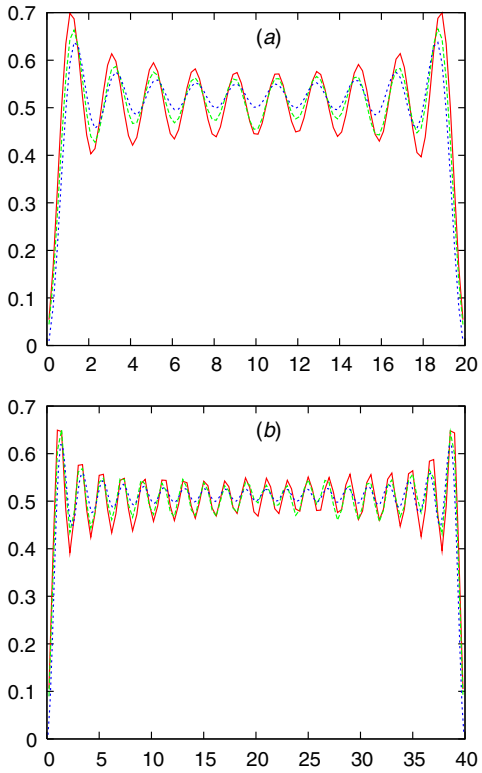

Figure 1. Density distribution of 10(*a*) and 20(*b*) spinless electrons in one dimensional box (red solid lines). Also shown are: interacting distinguishable particles (without the exchange; green dashed lines) and identical non-interacting particles (blue dot lines).

Table 1. Simulation parameters and computed energies for N interacting electrons in the external potential (1). Background charge density $\rho_0 = 0.5$ in all the cases. $E_{\rm el}$ is the potential energy of electron–electron interaction, $E_{\rm ex}$ is the energy of interaction with the external field, $E_{\rm kin}$ is the kinetic energy and $E_{\rm tot}$ is the total energy. Statistical uncertainty is given in parentheses.

Run	N	L	A	m	$E_{\rm el}$	$E_{\rm ex}$	$E_{\rm kin}$	$E_{\rm tot}$
1	10	20	0	–	11.057	−20.420	4.729	−4.635
					(0.002)	(0.002)	(0.005)	(0.007)
2	20	40	0	–	28.815	−54.357	8.995	−16.548
					(0.004)	(0.004)	(0.012)	(0.015)
3	9	20	1.0	10	8.232	−21.048	4.734	−8.081
					(0.004)	(0.004)	(0.01)	(0.012)
4	10	20	1.0	10	10.484	−23.818	6.103	−7.231
					(0.002)	(0.002)	(0.003)	(0.004)
5	11	20	1.0	10	13.840	−25.380	7.282	−4.258
					(0.002)	(0.002)	(0.006)	(0.008)
6	12	20	1.0	10	17.198	−26.883	8.768	−0.917
					(0.002)	(0.002)	(0.005)	(0.007)

distinguishable particles (without the exchange) and densities of non-interacting identical particles in a box are shown (the densities for non-interacting particles were built as a sum of N lowest one-particle densities).

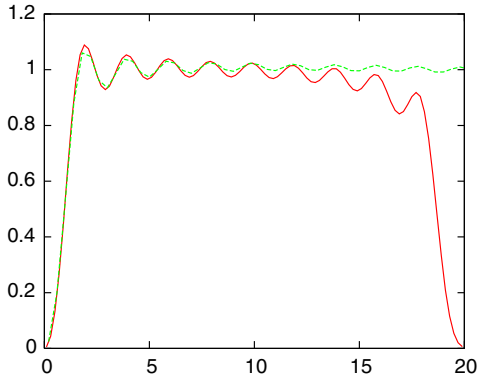

Figure 2. Pair correlation function for 10 (red solid line) and 20 (green dashed line) electrons in the field of uniform neutralizing background.

It is clearly seen that the density maxima are located at about equal distance from each other, due to the fact that the electrostatic electron–electron repulsion is counteracted by the potential (1) from the background charge. Electrons repeal each other both due to the electrostatic repulsion and the exchange interaction. Interaction and exchange effects amplify each other leading to higher oscillations of the electron density comparing to the cases when only exchange or only interaction effects are present. Still, oscillations of the density are not large and they are decreasing upon the increase of the system size, see figure 1(*b*). In the limit of an infinite system (but finite β), the single particle density is expected to tend to its average value.

Another insight into the properties of interacting electrons can be obtained by looking at the pair correlation function $g(x)$, which expresses probability to find two particles with distance x between them, normalized by the condition that the function is equal to 1 for particles distributed with a uniform probability. The pair correlation functions for 10 and 20 electrons (runs 1 and 2) are shown in figure 2. One can see that the correlation function is close to 1 for most of distances. Noticeable correlations exist only for neighbouring electrons, which cannot come close to each other, whereas for the next neighbours correlations are on the level of a few per cent.

The above described results were obtained when the electrons were in the field of a uniform background charge. Let us consider possible effect of their interactions with localized atoms which are mimicked by the second part of the potential (1).

In figure 3(*a*), the densities of 9–12 electrons in effective field of a 10-site lattice are displayed (runs 3–6 in table 1). Comparing to the case of a uniform background charge, the system of 10 electrons shows much better pronounced maxima and minima which is not surprisingly due to the form of the external potential with the amplitude $A = 1$. For $N = 10$, each electron is essentially localized around the corresponding 'atom'. Cases different from 10 number of electrons can now be interpreted as the appearance of 'conducting electrons' ($N = 11, 12$) or 'holes' ($N = 9$). One can observe in figure 3(*a*), that in the case of excess of electrons, additional electron density appears at the minima of the reference density corresponding to $N = 10$, while in the case of a hole ($N = 9$), the density disappears from the maxima of that curve.

In figure 3(*b*), the differences of the total electron density for 9, 11 and 12 electrons, and the reference density for 10 electrons are displayed. They can be interpreted as the charge density of a hole or of one or two conducting electrons, respectively. The striking result is a

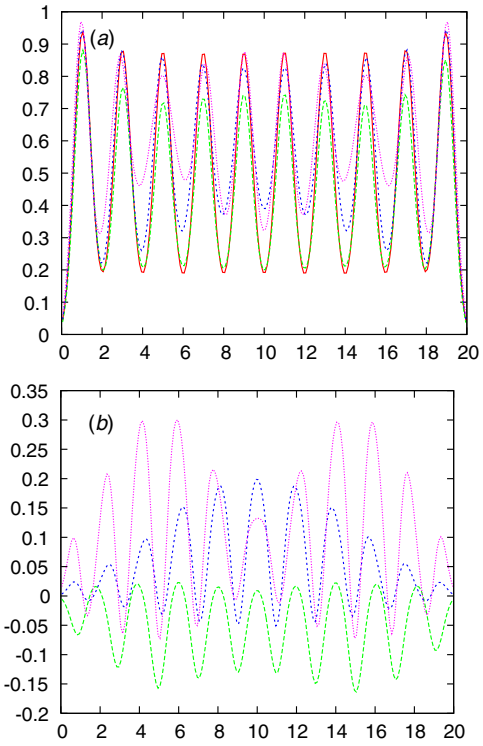

Figure 3. Density distribution for 10 (solid red line), 9 (green dash line), 11 (blue short dash line) and 12 (pink dot line) electrons in the external potential (1) with $m = 10$ wells of amplitude $A = 1$ (*a*) and differences of the density of 9, 11 and 12 electrons with the density of 10 electrons (*b*).

clearly different behaviour of the conducting electron density ($N = 11$), which is well centred in the middle of the system, and the density for the hole ($N = 9$) that is more delocalized and even has a tendency to form two maxima closer to the borders of the interval. It is tempting to note that the electron–hole asymmetry is a topic of current discussions [14–16] including their possible role in the superconductivity [14].

4. Conclusion

The examples presented here show that the PIMC approach can provide accurate computations of equilibrium properties of strongly interacting electron systems in one dimension, solely on the basis of the fundamental relationships of quantum mechanics. The PIMC method can thus become a power tool in investigation and understanding of such systems. It can be used for testing of analytical theories describing the properties of electrons in one-dimensional structures and semiconductors. For example, density functionals can be tested directly since the electron density and the energy can be readily obtained for a given external potential. Spin effects can be incorporated by considering exchange between spin-up and spin-down electrons separately [2]. It seems plausible that the considered approach would work for one-dimensional-like systems even if one considers three-dimensional space explicitly, with the motion along two other coordinates strongly restricted by an external potential. Though the weight function in this case will not be strictly positive, the path trajectories will likely be close

to the strictly one-dimensional ones, and the sign problem would not be too severe. This would provide even more realistic description of electrons in quantum-wire-like nanostructures.

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