Monte Carlo simulations of the electron short-range quantum ordering in Coulomb systems and the ‘fermionic sign problem’

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1. Introduction

One of the cornerstone challenges in the path integral Monte Carlo (PIMC) simulations of fermionic systems is the ‘sign problem’. The ‘sign problem’ arises from the antisymmetrization of the fermion density matrix [1–4] resulting for thermodynamic values being the small...
differences of large numbers associated with even and odd permutations and the exponential
growth of the statistical errors in PIMC simulations. To overcome this issue a lot of approaches
have been developed, but the ‘fermionic sign problem’ for strongly correlated fermions has not
been completely solved during the last fifty years. In [5, 6] the Wigner formulation of quan-
tum mechanics has been used avoid the antisymmetrization of matrix elements and hence the
’sign problem’. This approach allows to realize the Pauli blocking of fermions, however it is
not applicable at high degeneracy.

In [7] to reduce the ‘fermionic sign problem’, the restricted fixed-node path-integral Monte
Carlo (RPIMC) simulations of the uniform electron gas (UEG) at finite temperature has been
developed. In RPIMC to avoid the ‘sign problem’ only positive permutations are taken into
account, so the accuracy of the results is unknown and the error is difficult to quantify. More
interesting approaches are the new permutation blocking path integral Monte Carlo (PB-PIMC)
and the configuration path integral Monte Carlo (CPIMC) methods [8]. The main idea of
CPIMC is to evaluate the density matrix in the space of occupation numbers. However it
turns out that the CPIMC method exhibits also the ‘sign problem’. In PB-PIMC the sum
over permutations is presented in the form of a determinant, which can be calculated by the
direct highly accurate methods of linear algebra allowing to reduce the sign problem. How-
ever the disadvantage of this method is that the determinants are the sign-altering functions
worsening the accuracy of the PIMC simulations and giving rise to the ‘sign problem’ of
determinants.

In this paper we continue the series of our publications [3, 4, 9, 10] on the improvements
of the PIMC approach for strongly correlated systems of fermions and degenerate plasma media.

The paper [9] contains two main modifications in comparison with [3, 4]. First, we included
long-range Coulomb effects via Ewald summation with angular averaging as proposed by
Yakub and Ronchi [11]. Second, we improved the treatment of fermionic exchange interac-
tion of the strongly degenerated electrons, for cases where the electron thermal wavelength
exceeds the length of the Monte Carlo cell. We accounted for not only exchanges between
particles in the main Monte Carlo cell but also with particles in the nearest neighbor cells.
This additional interaction had a drastic effect on the computed energy. Good accuracy was
demonstrated for the limiting case of the ideal Fermi gas, for which analytical results are very
well-known.

The continuation of this work was published in the paper [10], which contained two addi-
tional alterations. The first one is attributed to the improved treatment of exchange interaction
in comparison with [9] achieved by the proper change of variables. This procedure modifies
the path integral measure and exchange determinant, which takes the form of the Gram deter-
minant being always non-negative. The latter is very important for the convergence of Monte
Carlo calculations. The second improvement is the angular averaging of the exchange deter-
minant describing the fermionic exchange interaction not only between particles in the main
Monte Carlo cell but also with particles in the periodic neighbor cells. This approach does not
meet the ‘sign problem’ and demonstrates good accuracy both for the strongly coupled and the
ideal Fermi systems.

In this article to improve the accuracy of the mentioned above approach and to account
for the interference effects of the Coulomb and exchange interactions of electrons we have
developed a new path integral representation of density matrix, in which interaction is included
in the exchange determinant.

Using this representation we have developed a modified fermionic path integral Monte Carlo
approach (MFPIMC) and have detected and investigated a short-range quantum ordering of
electrons. This effect is confirmed by the electron–electron pair distribution functions for two-
component plasma (TCP) and uniform electron gas (UEG). The observed ordering is caused
by the interaction of electrons with positively charged exchange holes and the excluded volume resulting in the formation of exchange-correlation excitons [12, 13]. More intuitively one can argue that the exclusion principle pushes other electrons with the same spin away from a reference electron, leaving a positive charge and an opposite spin [12, 13]. This positive charge with spin compensates the charge and spin of the reference electron. Since this phenomenon occurs over atomic distances, the electron–electron repulsion is reduced dramatically. Such short-range screening validates a simple Fermi-liquid model of metals which assumes nearly-free electrons.

Here obtained from the MFPI M pair distribution functions charge estimation of the exchange hole shows that its average positive charge is equal to the electron charge making the exchange-correlation exciton neutral as expected in [12, 13]. The obtained internal energy is a bit larger than available in the literature as the short-range ordering does not give noticeable contributions to integral thermodynamic characteristics. Such fine effect has not been observed earlier in standard PIMC simulations.

2. Many-particle density matrix

Let us start from a neutral Coulomb system of quantum electrons and positive classical (for simplicity) charges with the Hamiltonian, \( H = \hat{K} + U_t \), containing the kinetic \( \hat{K} \) and Coulomb interaction energies, \( U_t = U_{tp} + U_{ee} + U_{re} \). Thermodynamic properties in the canonical ensemble with a given temperature \( T \) and fixed volume \( V \) are fully described by the density operator \( \hat{\rho} = e^{-\beta H} \), with the partition function \( Z(N_e, N_p, V; \beta) = \sum_n \int_V dx \rho(x, \sigma; \beta) \), where \( \beta = 1/k_B T \), and \( \rho(x, \sigma; \beta) = \langle x | e^{-\beta H} | x \rangle \) denotes the diagonal elements of the density matrix in the coordinate representation. Here \( x = \{x_e, x_p\} \) (in units of thermal wavelengths \( \lambda_T = \sqrt{\frac{2\pi k_B T}{m}} \)) are the spatial coordinates of electrons and positive charges i.e. \( x_e = \{x_{1,e}, \ldots, x_{N_e,e}\} \) and \( \sigma = \{\sigma_1,e, \ldots, \sigma_{N_p,e}\} \) are the spin degrees of freedom of the electrons.

Generally the exact matrix elements of the density matrix of interacting quantum systems is not known, but can be constructed using a path integral representation [1–3] based on the operator identity, \( e^{-\beta H} = e^{-\beta K} e^{-\beta U} \cdots e^{-\beta U} \) (\( \epsilon = \beta / M \)), that involves \( M \) identical high-temperature factors with a temperature \( MT \):

\[
\rho(x, \sigma; x, \sigma; \beta) = \langle x | e^{-\beta H} | x \rangle \approx \sum_{P} (-1)^{P} S(\sigma, P\sigma) \times \prod_{m=0}^{M-1} e^{-\beta U_m(x) e^{-\beta K} | P\sigma \rangle} = \int \prod_{1}^{M} dx^{(1)} \cdots dx^{(M-1)} 
\]

\[
\times \exp \left\{ -\sum_{m=0}^{M-1} \left[ \frac{\pi}{2} | x^{(m)} - x^{(m+1)} |^2 + \epsilon U(x^{(m)}) \right] \right\} \operatorname{det} | \Psi(x) |, \quad (1)
\]

where index \( m = 0, \ldots, M \) labels the off-diagonal matrix elements of the high-temperature density matrices. Here each high-temperature factor has been presented in the form \( \langle x^{(m)} | e^{-\beta H} | x^{(m+1)} \rangle \approx \langle x^{(m)} | e^{-\beta K} | x^{(m+1)} \rangle \rho_0^{(m)} \) with the error of order \( 1/M^2 \), arising from neglecting the commutator \( \epsilon^2 / 2 [K, U_t] \). In the limit \( M \to \infty \) the error of the whole product is equal to zero \( (\propto 1/M) \), resulting in exact path integral representation of the partition function. Now each particle is presented by a trajectory consisting of a set of \( M \) coordinates \( x^{(m)} \). The sum is over all permutations with parity \( \kappa_{P} \). The spin gives rise to the spin part of the density matrix \( S \) with exchange effects accounted for.
by the permutation operator $P$ acting on the electron coordinates in $x^{(M)}$ and spin projections $\sigma$. Here we have assumed that in the thermodynamic limit the main contribution in the sum over spin variables comes from the term related to equal number ($N_e/2$) of electrons with the same spin projection $[3, 4]$, so the sum over permutation gives the product of determinants:

$$\det \|\Psi(x)\| = \det \|e^{-\frac{x^2}{2} - \frac{m^2}{2}}\|^{N_e/2} \det \|e^{-\frac{x^2}{2} - \frac{m^2}{2}}\|^{N_e(2N_e+1)}.$$  

The density matrix elements involve an effective pair interaction $U = \frac{1}{2}\sum_{\kappa\tau} \Phi_{\kappa\tau}$, which is approximated by the Kelbg potential given by the expression:

$$\Phi_{ab}(x_{ab}; \epsilon) = \frac{\epsilon_{ab}\epsilon_{ab}}{\lambda_{ab} x_{ab}} \left[1 - e^{-x^2_{ab} + \sqrt{\pi}x_{ab}\{1 - \text{erf}(x_{ab})\}}\right].$$

Here $\lambda_{ab} = |q_{ab} - q_{ab}| \Lambda_4$, $\Lambda_4 = 2\pi \hbar^2\epsilon/m_{ab}$, $1/m_{ab} = 1/m_a + 1/m_b$, $\Lambda_4^2 = 2\pi \hbar^2\epsilon/m_a$ and erf$(x)$ is the standard error function. At $x_{ab} \geq \lambda$, the Kelbg potential coincides with the Coulomb one, but is finite at $x_{ab} \rightarrow 0$ due to its quantum nature $[2–4]$.

A disadvantage of equation (1) is the sign-altering determinant $\det \|\Psi(x)\|$, which is the reason of the ‘sign problem’ worsening the accuracy of the PIMC simulations. To reduce the ‘sign problem’ let us replace the variables of integration $x^{(m)}$ by $q^{(m)}$ for any given permutation $P$ by the substitution: $x^{(m)} = (Px - x)\frac{m}{M} + x + q^{(m)}$ $[10]$. After some transformations, the diagonal matrix elements of the density matrix can be rewritten in the form of path integral over ‘closed’ trajectories $\{q^{(0)}, \ldots, q^{(M)}\}$ with $q^{(0)} = q^{(M)} = 0$ (see appendix for details):

$$\rho(x, \sigma; x, \sigma; \beta) \equiv \int dq^{(1)} \ldots dq^{(M-1)} \exp[-U_E] \times \left\{ \sum_\sigma \sum_P (\pm 1)^{\sigma_P} \right. \times S(\sigma, P\sigma) \exp \left[-\pi\frac{|P_x - x|^2}{M} - \sum_{m=0}^{M-1} \pi |\eta^{(m)}|^2 - \Delta U_P \right] \} \right.$$  

$$\approx \int dq^{(1)} \ldots dq^{(M-1)} \exp \left\{-\sum_{m=0}^{M-1} \pi |\eta^{(m)}|^2 - U_E \right\} \det \|\psi(x)\|, \quad (2)$$

where $\det \|\psi(x)\| = \det \|\phi_{kl}\|^{N_e/2} \times |\det \|\phi_{kl}\|^{N_e/(2N_e+1)}$,

$$\phi_{kl} = \exp\left\{-\pi |r_{kl}|^2/M \right\} \times \exp \left\{-\sum_{m=0}^{M-1} \left( \epsilon \Phi \left( r_{kl} + q^{(m)} \right) \right) \right\}$$

$$- \epsilon \Phi \left( r_{kl} + q^{(m)} \right) \right\} \quad (3)$$

and

$$U_E = \exp \left\{-\sum_{m=0}^{M-1} \epsilon U (x + q^{(m)}) \right\},$$

$$\Delta U_P = \sum_{m=0}^{M-1} \epsilon U (Px - x)\frac{m}{M} + x + q^{(m)} - U_E.$$
Here we introduced the following notation for the coordinate vectors: \( \eta^{(m)} \equiv q^{(m)} - q^{(m+1)} \), \( r_{li} \equiv (x_k - x_l), (k, l = 1, \ldots, N_e) \).

The approximation given by equation (2) reproduces both limits of the highly degenerate and non-degenerate systems of fermions. In the classical limit due to the factor \( \exp[-\pi |P x - x|^2 / M] \) the main contribution comes from the identical permutation and the differences of potential energies in the exponents of equations (2) and (3) are equal to zero. At the same time for highly degenerate plasma, where the thermal wavelength is larger than the average interparticle distance and trajectories are highly entangled the potential energy in equation like (2) weakly depends on permutations, that enables to replace all permutations by the identical one \( E \) [3–6]. At intermediate degeneracies the determinant in equation (2) accounts for the interference effects of the Coulomb and exchange interactions of electrons, that allows also to reduce the ‘fermionic sign problem’ by making use of direct methods to calculate the determinants. For better understanding of the mathematical structure of equation (2) let us consider two spinless fermions \( N_e = 2 \left( q^{(m)}_{12} = q^{(m)}_1 - q^{(m)}_2, \det \| \psi(x) \| = 1 - \phi_{12} \phi_{21} \) )

\[
\rho(x_1, x_2) \equiv \int dq^{(1)} \ldots dq^{(M-1)} \exp \left[ - \sum_{m=0}^{M-1} \pi |\eta^{(m)}|^2 \right] \times \left\{ \exp \left[ -\epsilon \Phi \left( r_{12} + q^{(m)}_{12} \right) \right] - \exp \left[ -\frac{\pi}{M} 2 r_{12}^2 \right] - \epsilon \Phi \left[ r_{12} \left( 1 - 2m/M \right) + q^{(m)}_{12} \right] \right\}. \tag{4}
\]

One can easily check that equation (4) obtained from the approximation (2) coincides with the exact density matrix of two fermions.

\[
\rho(x_1, x_2) \equiv \int dq^{(1)} \ldots dq^{(M-1)} \left\{ \exp \left[ - \sum_{m=0}^{M-1} \pi |\eta^{(m)}|^2 \right] + \epsilon \Phi \left( r_{12} + q^{(m)}_{12} \right) \right\} - \exp \left[ -\frac{\pi}{M} \frac{r_{12}^2}{2} - \frac{\pi}{M} \frac{r_{21}^2}{2} \right] - \sum_{m=0}^{M-1} \left[ \pi |\eta^{(m)}|^2 + \frac{\epsilon}{2} \Phi \left( \frac{r_{21}^2}{M} + r_{12} + q^{(m)}_{12} \right) \right] + \frac{\epsilon}{2} \Phi \left( \frac{r_{12}^2}{M} + r_{21} + q^{(m)}_{12} \right) \right\}. \tag{5}
\]

3. Simulation details

In TCP all charges are correlated due to interaction, while in our model of UEG the positive particles are uncorrelated to simulate the neutralizing background [9, 10]. Here the density of electrons is characterized by the Brueckner parameter \( r_s = a / a_0 \), where \( a = [3 / (4\pi n_e)]^{1/3}, n_e \) is the electron density and \( a_0 \) is the Bohr radius. Temperature will be given in Rydberg units of energy or the Fermi energy \( \Theta = T / E_F \). In our MFPIMC simulations we used the Metropolis algorithm [2–4] and varied both the particle number in the range \( N_e = 30, \ldots, 50 \), and the number of high-temperature factors in the range \( M = 20, \ldots, 30 \) to check the convergence of
calculated results. To analyze the influence of interparticle interaction on the exchange properties of fermions we have compared internal energy and pair distribution for the exchange matrix $\|\phi_{kt}\|$ given by (3) (marked by A1) with those given by expression $\tilde{\phi}_{kt} \approx e^{-\pi |x_k - x_t|^2}$ (marked by A2).

4. Pair distribution functions, short range ordering and charge neutrality

Let us start from the physical analysis of the spatial arrangement of electrons and positive particles, by studying the pair distribution functions (PDF) $g_{ab}(R)$ defined as:

$$g_{ab}(|R_1 - R_2|) = \left(\frac{V}{N}\right)^2 \sum_{\sigma} \sum_{i,j \neq f} \delta_{a_i,a} \delta_{a_j,b} \frac{1}{Z} \int dr \delta(R_1 - r_i) \delta(R_2 - r_j) \rho(x, \sigma; \beta), \quad (6)$$

where $a$ and $b$ are the sorts of particles (electron or positive charge). PDFs depend only on the difference of particles coordinates $R = |R_1 - R_2|$ because of the translational invariance of the system. The product $R^2 g_{ab}(R)$ is proportional to the probability to find two particles at a distance $R$. The PDFs averaged over spin of electrons are shown in figure 1(a). In a non-interacting classical system $g_{ep}(R) = 8_{pp} \equiv 1$, whereas the interparticle interactions and quantum statistics result in a redistribution of particles (see lines 1, 2, 5, 6 in figure 1(a)). For UEG the rigid neutralizing background is simulated as an ideal gas of uncorrelated classical positive charges uniformly distributed in space, so $g_{pp}$ and $g_{ep}$ are identically equal to unity, that is demonstrated by lines 3 and 4 in figure 1(a).

An interesting result of MFPIMC calculations is the peak in the same spin $g_{ee}$ at an interparticle distance of the order of the electron thermal wavelength (see figure 1(b)). At a temperature $T/Ry = 3$ for TCP and UEG lines 7 and 8 show $g_{ee}$ related to the case A1, while lines 9 and 10 present $g_{ee}$ corresponding to the case A2. Here electron thermal wavelength $\lambda_e \approx 1a_0$ at $T/Ry = 12$ and $\lambda_e \approx 2a_0$ at $T/Ry = 3$. Small oscillations on the PDFs are the Monte-Carlo statistical error.

Let us consider the physical reasons of the drastic difference in behavior of $g_{ee}$ related to the cases A1 and A2. The comparison of PDFs $g_{ee}$ and $g_{ep}$ allows us to conclude that compact three-particle complexes consisting of two electrons and a positive particle have been formed at interparticle distances of the order of the electron thermal wavelength. The charge of such
complex can be estimated using the integrals of probabilities of finding two particles of the sorts \( a \) and \( b \) at a distance \( r \) apart \( (\sim r^2 \, g_{ab}(r)) \) by the formula

\[
Z_{\text{tot}}(\tilde{r}) \sim \int_{\tilde{r}}^{\tilde{r}+\lambda_e} 4\pi r^2 (g_{ep}(r) - g_{ee}(r)) \, dr
\]

for \( \tilde{r} \sim \lambda_e \).

Figure 2 shows the TCP and UEG PDFs and the total exciton’s charge distribution versus the distance from one electron and confirms exciton electric neutrality, since the average charge of a positively charged hole tends to zero due to the presence the second electron at \( \tilde{r} \rightarrow \lambda_e \). In the exchange hole on average a positive charge prevails at small distances from the electron, but then is compensated at a distance of order of the wavelength of the electron (see figure 2.) So we can conclude that the charge of the exchange hole is equal to charge of electron. The peak can be associated with the exchange-correlation excitons \([12, 13]\) arising due to the occurrence of the exchange positively charged hole (see blue and red \( g_{ep} \) in figure 1) and the excluded volume effect \([14]\). This effect is consequence of the interference effects of Coulomb and exchange interactions of electrons, taken into account by the determinant in the equation (2). Contrary to approximation A2 the expression A1 for the exchange matrix accounts for more accurately the Coulomb and Fermi repulsion of electrons resulting in the occurrence of the peak in \( g_{ee} \).

5. Density–temperature range of the exciton existence

Figure 3(a) allows to estimate the density and temperature range of the exchange-correlation exciton existence. In the classical limit \( (\theta = T/E_F \geq 4) \) and at high degeneracy \( (\theta \leq 0.5) \) excitons disappear, while in the intermediate region we can see their generation and decay. From the physical point of view the exchange-correlation excitons can exist when the thermal wave of electron is smaller or order of the average interparticle distance, but in the classical limit excitons are also destroyed (at high temperature and low density). Let us stress that the formation of exchange-correlation excitons is possible only for electrons with the same spin projections (see figure 3(a)).

Figure 3(b) shows that approximation A2 cannot reproduce exchange-correlation excitons in spite of reproducing the exchange-correlation and correlation electron holes for the same and opposite spins respectively.

Let us note that under these conditions the main contribution to the thermodynamic of fermions comes from repulsive pair exchange interactions \([5, 6]\). However equation (2) with case A1 exactly reproducing the two fermion density matrix contrary to the case A2 and
Figure 3. The UEG pair distribution functions obtained according to equation (2) for cases A1 (a) and A2 (b) at $r_s = 1$ and different $\theta$. The PDF corresponding to the same/opposite spin projections ($g_{ee}/g_{oo}$) are presented by the solid/dashed lines respectively. The UEG PDFs $g_{ee}$, $g_{pp}$ are identically equal to unity. Small oscillations of the PDF are the Monte-Carlo statistical error.

Table 1. Internal energy $E$/Ha.

| $\Theta$ | Case A1 | Case A2 | Reference [7] |
|----------|----------|----------|----------------|
| 0.5      | 1.41     | 1.29     | 1.32           |
| 1        | 2.68     | 2.57     | 2.61           |
| 2        | 5.42     | 5.33     | 5.35           |
| 4        | 11.34    | 10.79    | 10.87          |

that is the reason of the discrepancy in obtained results. So accounting for interference effects of the Coulomb and exchange interactions in matrix $\psi$ is crucial for description of the exchange-correlation excitons.

6. Internal energy

Calculations of the internal energy for UEG has been done by the energy estimator [9, 10]. As example, the obtained results for cases A1 and A2 in equation (2) in comparison with [7] are presented in table 1 at $r_s = 1$. The internal energy $E$ and PDFs $g_{ee}$ for the case A1 are larger than those for case A2 and in [7]. The difference is noticeable but not very big as the product $r^2 g_{ee}(r)$ reduces contributions at small interparticle distances in the integral thermodynamic characteristics.

7. Discussion

In this paper to overcome the ‘sign problem’ of determinants we have developed an approximation of the matrix elements of the density matrix for fermion system, in which the exchange determinant takes the form of non-negative Gram determinant. To improve the accuracy of this approximation and to account for the interference effects of the Coulomb and exchange interactions of electrons we have developed a new path integral representation of density matrix, in which interaction is included in the exchange determinant. Using this representation we have developed a modified fermionic path integral Monte Carlo approach (MFPIMC) and have revealed and investigated a short-range quantum ordering of electrons.
Approximation A2 is valid for a highly degenerate system [10]. In this case the determinant \( \psi(x) \) is equivalent to the Gram determinant \([15]\) \( \det(\langle \chi(x_i)|\chi(x_j)\rangle) \) of linearly independent system of \( N_e \) vectors \( \chi_p(x_i) = |e^{i[p\cdot x_i]}/\hbar| \) with the scalar product defined as \( \langle \chi(x_i)|\chi(x_j)\rangle = \int dp \ e^{-\vec{p}^2/2m} / \int dp \ e^{-\vec{p}^2/2m} = e^{-\pi\hbar^2/4M^2} \). The Gram determinant is always non-negative \([15]\) and allows to solve the ‘sign problem’ in PIMC simulations of fermions in the discussed approximation.

For comparison let us consider similar matrix elements \( e^{-\pi\hbar^2/4M^2} \) in the exchange determinants \( \det \Psi(x) \) in equation (1) used in the standard PIMC. Let us note that \( \psi(x) \) in equation (2) has a different structure in comparison with the matrix elements in \( \Psi(x) \), which are defined by the analogous scalar product but for the other set of \( 2N_e \) vectors \( |e^{i[p\cdot x_i^m]/\hbar}| \) and \( |e^{i[p\cdot x_i^m]/\hbar}| \).

The MF PIMC method for the exchange matrix \( \psi \) with \( \phi_{ik} \) given by equation (3) case A1 contrary to the less accurate case A2 demonstrates a short-range quantum ordering of electrons arising from the Coulomb interaction of electrons with positively charged exchange holes. This fine phenomenon is known in the literature \([12, 13]\) and is associated with the formation of exchange-correlation excitons which modify the pair correlations. Obtained results allow to estimate the density–temperature range of exciton existence and to demonstrate their electric neutrality. The problem of the exchange-correlation exciton is included by the Prof. Franz J. Himpsel in a collection of theory projects addressing long-standing questions in physics (see https://uw.physics.wisc.edu/himpsel/TheoryProjects.html).

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**Data availability statement**

The data that support the findings of this study are available upon reasonable request from the authors.

**Appendix. Derivation of the new path integral representation of the density matrix**

For simplicity let us prove equation (2) for spinless fermions. The generalization for fermions with spin degree of freedom is trivial. Equation (2) has been obtained in \([4–6]\) after replacing variables \( x^{(m)} \) by \( q^{(m)} \) for any given permutation \( P \) by the substitution \( x^{(m)} = (Px - x) \frac{2m}{\hbar^2} + x + q^{(m)} \) in the standard expression for the path integral representation of density matrix like in equation (1) \([1, 2]\).

Let us derive the new path integral representation of the density matrix. From the expression for potential energy \( \epsilon U \ (Px - x) \frac{2m}{\hbar^2} + x + q^{(m)} \) in equation (2) it follows that each coordinate of vector \( x_k \) may be changed by the term \( (x_{Pk} - x_k) \frac{2m}{\hbar^2} \) only if \( Pk \neq k \). The pair potentials relating to the identical permutation and the pair potentials relating to a non-identical one will be denoted further by symbols \( \Phi_{ik} = \epsilon \Phi(|r_{ik} + q^{(m)}_{ik}|) \) and \( \Phi_{ik} = \epsilon \Phi(|r_{ik} 2m + r_{ik} + q^{(m)}_{ik}|) \).
respectively. The difference of the matrix elements $\Delta \tilde{\Phi}_{lt} = \tilde{\Phi}_{lt} - \Phi_{lt}$ is non-zero only if the permutation changes the number $k$ or/and $t$ ($Pk \neq k$ or/and $Pt \neq t$). So the non-zero elements $\Delta \tilde{\Phi}_{lt}$ for any given permutation $P$ form rows and columns with correspondent numbers $k$ and $t$ (see for example in the tables A1 and A2 below).

In the sum over permutations in equation (2) every permutation $P$ is comprised of cyclic ones without common components [15]. So without the loss of generality we can consider only cyclic permutations. At this point we introduce an approximation allowing to reduce the ‘fermionic sign problem’ and to make use of the advantages of direct methods of linear algebra to calculate determinants describing the exchange interaction. We have replaced the pair potentials $\tilde{\Phi}_{lt}$ with $\Phi_{lt}$ in row $k$ and column $t$ except their intersection marked by stars $\times \Phi_{lt}$. So in the considered approximation in row $k$ and column $t$ all matrix elements $\Delta \tilde{\Phi}_{lt} = \tilde{\Phi}_{lt} - \Phi_{lt}$ are equal to zero except $\times \Delta \tilde{\Phi}_{lt}$. For example, tables A1 and A2 show these values for a simple permutation comprising from two non-trivial cyclic permutations and four identical cycles $P_{c} = (1, 3, 5), (4, 7), (2, 2), (6, 6), (8, 8), (9, 9)$ for 9 particles. As a result of this approximation we have for $P_{c}$:

$$\exp \left[-\pi \frac{|P_{c}x - x|^{2}}{M} - \Delta UP_{c} \right] \approx \phi_{13}^{*} \phi_{15}^{*} \phi_{47} \phi_{74}^{*},$$

where $\phi_{lt}^{*} = \exp \{-\pi |r_{lt}|^{2}/M\} \exp \{-\frac{1}{2} \sum_{m=0}^{M-1} \left( \epsilon \times \Delta \tilde{\Phi}_{lt} \right)\}, \phi_{lk}^{*} = 1$. (The product $\phi_{51}^{*} \phi_{15}^{*} \phi_{53}^{*}$ will be accounted for by a symmetric cycle like in $3 \times 3$ matrix).

The sum over all permutations gives the determinant $\det \|\psi(x)\|$ of matrix $\|\phi_{lt}\|$ in equation (2). From the physical point of view the determinant describes the interference effects of the Coulomb and the exchange interactions of electrons. Table A3 (as the final result) presents the matrix of all pair interactions related to the cyclic permutation $P_{c}$. 

Table A1. Initial matrix of pair potential for $P_{c}$.

|       | $\Phi_{12}$ | $\times \Phi_{13}$ | $\Phi_{14}$ | $\times \Phi_{15}$ | $\Phi_{16}$ | $\Phi_{17}$ | $\Phi_{18}$ | $\Phi_{19}$ |
|-------|-------------|-------------------|-------------|-------------------|-------------|-------------|-------------|-------------|
| $\Phi_{21}$ | 0          | $\Phi_{23}$       | $\Phi_{24}$ | $\Phi_{25}$       | $\Phi_{26}$ | $\Phi_{27}$ | $\Phi_{28}$ | $\Phi_{29}$ |
| $\times \Phi_{31}$ | 0          | 0                 | $\Phi_{34}$ | $\times \Phi_{35}$ | $\Phi_{36}$ | $\Phi_{37}$ | $\Phi_{38}$ | $\Phi_{39}$ |
| $\Phi_{41}$ | $\Phi_{42}$ | $\Phi_{43}$       | 0           | $\Phi_{45}$       | $\Phi_{46}$ | $\times \Phi_{47}$ | $\Phi_{48}$ | $\Phi_{49}$ |
| $\times \Phi_{51}$ | $\Phi_{52}$ | $\times \Phi_{53}$ | $\Phi_{54}$ | 0                 | $\Phi_{56}$ | $\Phi_{57}$ | $\Phi_{58}$ | $\Phi_{59}$ |
| $\Phi_{61}$ | $\Phi_{62}$ | $\Phi_{63}$       | $\Phi_{64}$ | $\Phi_{65}$       | 0           | $\Phi_{67}$ | $\Phi_{68}$ | $\Phi_{69}$ |
| $\Phi_{71}$ | $\Phi_{72}$ | $\Phi_{73}$       | $\Phi_{74}$ | $\Phi_{75}$       | $\Phi_{76}$ | 0           | $\Phi_{78}$ | $\Phi_{79}$ |
| $\Phi_{81}$ | $\Phi_{82}$ | $\Phi_{83}$       | $\Phi_{84}$ | $\Phi_{85}$       | $\Phi_{86}$ | $\Phi_{87}$ | 0           | $\Phi_{89}$ |
| $\Phi_{91}$ | $\Phi_{92}$ | $\Phi_{93}$       | $\Phi_{94}$ | $\Phi_{95}$       | $\Phi_{96}$ | $\Phi_{97}$ | $\Phi_{98}$ | 0           |

Table A2. Approximation of matrix of the pair potential differences for $P_{c}$.

|       | 0         | $\times \Delta \Phi_{13}$ | 0         | $\times \Delta \Phi_{15}$ | 0         | 0         | 0         | 0         |
|-------|-----------|-----------------------------|-----------|-----------------------------|-----------|-----------|-----------|-----------|
| 0     | 0         | 0                           | 0         | 0                           | 0         | 0         | 0         | 0         |
| $\times \Delta \Phi_{31}$ | 0         | 0                           | 0         | $\times \Delta \Phi_{35}$ | 0         | 0         | 0         | 0         |
| 0     | 0         | 0                           | 0         | 0                           | 0         | $\times \Delta \Phi_{47}$ | 0         | 0         |
| $\times \Delta \Phi_{51}$ | 0         | $\times \Delta \tilde{\Phi}_{53}$ | 0         | 0                           | 0         | 0         | 0         | 0         |
| 0     | 0         | 0                           | 0         | 0                           | 0         | 0         | 0         | 0         |
| 0     | 0         | 0                           | 0         | 0                           | 0         | 0         | 0         | 0         |
| 0     | 0         | 0                           | 0         | 0                           | 0         | 0         | 0         | 0         |
Table A3. Final matrix of pair potentials $\Phi_{kt}$ and $\tilde{\Phi}_{kt}$ for $P_c$.

| 0  | $\Phi_{12}$ | $\Phi_{13}$ | $\Phi_{14}$ | $\Phi_{15}$ | $\Phi_{16}$ | $\Phi_{17}$ | $\Phi_{18}$ | $\Phi_{19}$ |
|----|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| $\Phi_{21}$ | 0 | $\Phi_{23}$ | $\Phi_{24}$ | $\Phi_{25}$ | $\Phi_{26}$ | $\Phi_{27}$ | $\Phi_{28}$ | $\Phi_{29}$ |
| $\Phi_{31}$ | $\Phi_{32}$ | 0 | $\Phi_{34}$ | $\tilde{\Phi}_{35}$ | $\Phi_{36}$ | $\Phi_{37}$ | $\Phi_{38}$ | $\Phi_{39}$ |
| $\Phi_{41}$ | $\Phi_{42}$ | $\Phi_{43}$ | 0 | $\Phi_{45}$ | $\Phi_{46}$ | $\tilde{\Phi}_{47}$ | $\Phi_{48}$ | $\Phi_{49}$ |
| $\Phi_{51}$ | $\Phi_{52}$ | $\Phi_{53}$ | $\Phi_{54}$ | 0 | $\Phi_{56}$ | $\Phi_{57}$ | $\Phi_{58}$ | $\Phi_{59}$ |
| $\Phi_{61}$ | $\Phi_{62}$ | $\Phi_{63}$ | $\Phi_{64}$ | $\Phi_{65}$ | 0 | $\Phi_{67}$ | $\Phi_{68}$ | $\Phi_{69}$ |
| $\Phi_{71}$ | $\Phi_{72}$ | $\Phi_{73}$ | $\Phi_{74}$ | $\Phi_{75}$ | $\Phi_{76}$ | 0 | $\Phi_{78}$ | $\Phi_{79}$ |
| $\Phi_{81}$ | $\Phi_{82}$ | $\Phi_{83}$ | $\Phi_{84}$ | $\Phi_{85}$ | $\Phi_{86}$ | $\Phi_{87}$ | 0 | $\Phi_{89}$ |
| $\Phi_{91}$ | $\Phi_{92}$ | $\Phi_{93}$ | $\Phi_{94}$ | $\Phi_{95}$ | $\Phi_{96}$ | $\Phi_{97}$ | $\Phi_{98}$ | 0 |

Due to this approximation the particles from any given cycle interact with other particles with the pair potentials $\Phi_{kt}$ instead of $\tilde{\Phi}_{kt}$, while along the cyclic path the particle interaction is described by $\tilde{\Phi}_{kt}$. The number and length of the cycles giving the main contribution to the thermodynamics of the fermionic system depend on the degeneracy and can be very large or small.

At this perturbation in potential energy ($\Phi_{kt}$ instead of $\tilde{\Phi}_{kt}$) the change in corresponding free energy is of order

$$n_e \lambda^2 / 2 \int dr_{12} \int d(q_{12}^{(1)}, \ldots, d(q_{12}^{(M-1)}) g_{ee}(r_{12}, q_{12}^{(1)} \ldots q_{12}^{(M-1)})$$

$$\times \left( \exp \left( - \sum_{m=0}^{M-1} \epsilon \Delta \tilde{\Phi}_{12} \right) - 1 \right) \sim n_e \lambda^3 / 2 g_{ee}((n_e \lambda^3)^{-1/3})(-\beta \Delta \tilde{\Phi}((n_e \lambda^3)^{-1/3}))$$

and can be neglected for small $\Delta \tilde{\Phi}$ and $n_e \lambda^3 \ll 1$. Here $\beta e^2 / \lambda_e = \sqrt{\beta R_y / \pi}$ and $g_{ee}$ is the pair distribution function. This estimation can be obtained within the generalization of the Mayer expansion technique for strongly coupled systems of particles (by the so-called algebraic approach) [16, 17].

At a moderate degeneracy ($n_e \lambda^3 \lesssim 1$) because of the Fermi repulsion the main contribution to the exchange determinant in (2) is given by the pair exchange blocks [5, 6]. Let us note that under this conditions the Laplace expansion allows to approximate determinant in (2) by the product of the two particle exchange blocks (det $\psi(x)$) $\sim 1(1 - \psi_{12}(\phi_{12}))$ coinciding with exact two particles ones (5). So developed approximation of the density matrix (2) is correct at moderate degeneracy and has the correct asymptotic behavior in the low degeneracy limit.

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