Total and correlation energy of the uniform polarized electron gas at finite temperature: Direct path integral simulations

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Abstract. The uniform electron gas (UEG) at finite temperature has recently attracted substantial interest due to the experimental progress in the field of warm dense matter. To explain the experimental data accurate theoretical models for high density plasmas are needed which crucially depend on treatment of quantum effects in electron–electron interaction as well as in the interaction of electrons with uniform positive background. To comply with these requirements we have developed the new quantum path integral model of the UEG and present the results of related direct path integral Monte-Carlo (DPIMC) simulations. Contrary to the known in literature approaches treating the electron–background interaction classically our simulations take into account the quantum effects in this interaction. We have observed very good agreement with known in literature results only up to moderate densities when the ratio of the average interparticle distance to the Bohr radius is of order four \(r_s \geq 4\) and observe deviations for higher densities. At very high electron density \(r_s \approx 1\) presented in literature approaches as well as our simulations are problematic due to the strong degeneracy of electrons and increasing fermion sign problem.

1. Introduction
The neutral uniform electron gas (UEG) or jellium is a quantum mechanical model of interacting electrons where the positive charges (e.g. atomic nuclei of a solid) are assumed to form a uniform in space charge background that assures overall charge neutrality but which is not treated microscopically. The model allows one to focus on the effects that occur due to the quantum nature of electrons and their repulsive interactions. The artificial and structureless background charge interacts with itself and the electrons. The properties of the electron gas are a crucial ingredient to correctly describe dense plasmas as well as the electron gas in metals.

Accurate data for the electron gas at zero temperature have been provided long ago by quantum Monte Carlo simulations [1] and have been massively used in density functional calculations. In the mean time new and improved ground state data have appeared, the most accurate ones, apparently, being the configuration interaction Monte Carlo data [2,3]. However, these are all restricted to zero temperature and not applicable to highly excited systems such as warm dense matter.
The extension of ab initio simulations to finite temperature is possible using the path integral
Monte Carlo (PIMC) technique, e.g. [4–10], and many results have been obtained for fermions
in the recent two decades, including correlated electrons in quantum dots, e.g. [11,12] or dense
plasmas, e.g. [13–17]. Only recently PIMC simulations were applied to the electron gas at finite
temperature. Brown et al presented restricted path integral Monte Carlo (RPIMC) results that
used the fixed node approximation [18] and covered a broad parameter range of the homogeneous
electron gas. A key problem of these data is that the accuracy of the results at high degeneracy
is unknown since the fixed nodes used in the RPIMC simulations carry a systematic error that
is difficult to quantifi. The use of the ideal gas nodes appears to be problematic for the nonideal
quantum Fermi gas (moderate $r_s$), where interaction effects may be relevant, as was shown for
the case of hydrogen by Militzer et al [13,19]. At the same time these nodes are not able to
reproduce the ideal Fermi gas limit, as was proven by one of us [20,21].

Another novel treatment of fermionic sign problem has been recently proposed in [22–25]. A
combination of these new concepts with the DPIMC approach of the present work and RPIMC
should allow one to achieve reliable theoretical predictions for the uniform electron gas in the
entire parameter range in the near future.

Therefore, the motivation of the present work is to perform new independent first-principle
direct fermionic PIMC simulations and compare them to the earlier results. To this end we
make use of a DPIMC approach that was developed several years ago and successfully applied
to dense hydrogen [26–28], hydrogen-helium mixtures [29,30], to the electron-hole plasmas in
semiconductors [31,32] and to the nonideal quark–gluon plasma [33,34].

In this paper we demonstrate the improved treatment of fermionic exchange by comparison
with the analytical data for the ideal Fermi gas. Our comparison with the RPIMC data reveals
very good agreement for low and moderate densities, $r_s \geq 4$ for the non ideal polarized electron
gas and deviations for higher densities at temperatures below the Fermi temperature.

2. Path integral representation

Classical simulations of Coulomb systems face the problem of an unlimited increase of the
interaction energy at small distances. Quantum simulations such as path integral Monte Carlo
avoid the Coulomb divergences in a natural way. This has been demonstrated before for PIMC
simulations of two-component electron-ion plasmas e.g. [27,28] and electron-hole plasmas [32].
Here we adapt these simulations to jellium by treating it as the limiting case of the neutral
two-component plasma ($N_e = N_p = N$) where, at the end, the background component (the
ions) will be treated as non-interacting.

Let us start from a quantum two-component Coulomb system of electrons and positive charges
in equilibrium with the Hamiltonian, $H = K + U^c$, containing kinetic energy $K$ and Coulomb
interaction energy contributions, $U^c = U^{c}_{pp} + U^{c}_{ee} + U^{c}_{ep}$. The thermodynamic properties in
the canonical ensemble with given temperature $T$ and fixed volume $V$ are fully described by the
density operator $\hat{\rho} = e^{-\beta \hat{H}}$, with the partition function

$$Z(N_e, N_p, V; \beta) = \frac{1}{N!_eN!_p} \sum_\sigma \int_V dq \rho(q, \sigma; \beta)$$

where $\beta = 1/k_B T$, and $\rho(q, \sigma; \beta)$ denotes the diagonal elements of the density matrix in
coordinate representation at a given value $\sigma$ of the total spin. In (1), $q = \{q_e, q_p\}$ and $\sigma = \{\sigma_e\}$
are the spatial coordinates of electrons and positive charges and spin degrees of freedom of the
electrons, i.e. $q_e = \{q_{1,e} \ldots q_{N_e,e}\}$ and $\sigma_e = \{\sigma_{1,e} \ldots \sigma_{N_e,e}\}$. In order to calculate
thermodynamic functions, the logarithm of the partition function has to be differentiated with
respect to thermodynamic variables. For example, for internal energy it follows $\beta E = -\frac{\partial \ln Z}{\partial \beta}$. 
The exact density matrix of interacting quantum systems is not known (particularly for low temperatures and high densities), but can be constructed using a path integral approach [4] based on the operator identity, \( e^{-\beta \hat{H}} = e^{-\Delta \beta \hat{H}} e^{-\Delta \beta \hat{H}} \ldots e^{-\Delta \beta \hat{H}} \), \( \Delta \beta = \beta/(n+1) \) that involves \( n+1 \) identical high-temperature factors with temperature \( (n+1)T \), which allows us to rewrite the integral in (1)

\[
\sum_{\sigma} \int dq^{(0)}(0) \ldots dq^{(n)}(0) \rho^{(1)} \ldots \rho^{(n)} \times \\
\sum_{P_\sigma} (\pm 1)^{\kappa_{P_\sigma}} S(\sigma, \hat{P}_e) \times \hat{P}_e \rho^{(n+1)} | q^{(n+1)} = q^{(0)}, \sigma' = \sigma \rangle.
\]

The spin gives rise to the spin part of the density matrix \( \rho \) with exchange effects accounted for by the permutation operator \( \hat{P}_e \) acting on the electron coordinates \( q^{(n+1)} \) and spin projections \( \sigma' \). The sum is over all permutations with parity \( \kappa_{P_\sigma} \). Equation (2) involves the off-diagonal high-temperature density matrices, \( \rho^{(l)} \equiv \rho(q^{(l-1)}, q^{(l)}; \Delta \beta) = \langle q^{(l-1)}(0) e^{-\Delta \beta \hat{H}} q^{(l)}(0) \rangle \), where \( l = 1 \ldots n+1 \). Accordingly, each particle is represented by a set of \( n+1 \) coordinates ("beads"), i.e. the whole configuration of the particles is represented by a \( 3(N_e + N_p)(n+1) \)-dimensional vector \( \tilde{q} \equiv \{ q_{1,e}^{(0)}, \ldots q_{1,e}^{(n+1)}; q_{2,e}^{(0)} \ldots q_{2,e}^{(n+1)}; \ldots q_{N_e,e}^{(0)}; q_{1,p} \ldots q_{N_p,p}^{(0)}; \ldots q_{N_p,p}^{(n+1)} \} \).

To determine the energy in the path integral representation (2) each high-temperature density matrix in product has to be differentiated [9, 28]. It is straightforward to show that using perturbation theory due to the small parameter \( \Delta \beta \) in each factor our final result for the energy is

\[
\beta E = \frac{3}{2} (N_e + N_p) + \frac{1}{Z} \frac{1}{\lambda_p^N \lambda_e^{n+1}} \sum_{s=0}^{N_e} \int dq^{(n)}(0) \ldots dq^{(n)}(0) \rho_s(q^{(0)} s) | \eta^{(1)} s \ldots \eta^{(n)} s, \beta \rangle \\
\times \left\{ \sum_{l=0}^{n} \left[ \sum_{k=1}^{N_p} \sum_{l=1}^{N_e} \Phi_{ep}(|x_{kl}^{(l)}|) + \sum_{k < l}^{N_e} \Phi_{ee}(|r_{kl}^{(l)}|) + \sum_{k < l}^{N_p} \Phi_{pp}(|q_{kl}^{(l)}|) \right] \\
+ \sum_{l=1}^{n} \left[ \sum_{k=1}^{N_p} \sum_{l=1}^{N_e} D(x_{kl}^{(l)}) \frac{\partial \Delta \beta \Phi_{ep}}{\partial |x_{kl}^{(l)}|} + \sum_{k < l}^{N_e} C(r_{kl}^{(l)}) \frac{\partial \Delta \beta \Phi_{ee}}{\partial |r_{kl}^{(l)}|} + \sum_{k < l}^{N_p} C(q_{kl}^{(l)}) \frac{\partial \Delta \beta \Phi_{pp}}{\partial |q_{kl}^{(l)}|} \right] \\
- \frac{1}{\det \langle |\psi^{(n)}_{kl}^s|_s | \rangle} \frac{\partial \det \langle |\psi^{(n)}_{kl}^s|_s | \rangle}{\partial \beta} \right\},
\]

with the definitions

\[
C(r_{kl}^{(l)}) = \frac{\langle r_{kl}^{(l)} | r_{kl}^{(l)} \rangle}{2 |r_{kl}^{(l)}|}, \quad C(q_{kl}^{(l)}) = \frac{\langle q_{kl}^{(l)} | q_{kl}^{(l)} \rangle}{2 |q_{kl}^{(l)}|},
\]

\[
D(x_{kl}^{(l)}) = \frac{\langle x_{kl}^{(l)} | x_{kl}^{(l)} \rangle}{2 |x_{kl}^{(l)}|}, \quad \Psi_{ab}(x) = \Delta \beta \frac{\partial \beta \Phi_{ab}(x, \beta')}{\partial \beta' \beta = \Delta \beta}.
\]

Here we introduced the following notation for the differences of two coordinate vectors

\[
q_{kl}^{(l)} \equiv q_{kl} - q_{kl}, r_{kl}^{(l)} \equiv q_{kl} - q_{kl} = x_{kl}^{(l)} + y_{kl}^{(l)}, q_{kl}^{(l)} = q_{kl} + y_{kl}^{(l)}, x_{kl}^{(l)} = x_{kl}^{(l)} + y_{kl}^{(l)}.
\]

\[
y_{kl}^{(l)} = \Delta \lambda_e \sum_{k'=1}^{l} r_{kl}^{(k')} + \Delta \lambda_p \sum_{k'=1}^{l} y_{kl}^{(k')}.
\]
It is also convenient to introduce dimensionless integration variables \( n^{(l)} = (\eta^{(l)}, \xi^{(l)}) \), where \( \eta^{(l)}_a = \kappa_a (q^{(l)}_a - q^{(l-1)}_a) \), for \( l = 1, \ldots, n \), and we use the dimensional factor \( \kappa_a^2 = m_a / (2\pi\hbar^2\Delta\beta) = 1/\lambda_{a,a}^2 \), for \( a = e, p \). The density matrices \( \rho_s \) appearing in (3) are given by

\[
\rho_s = C_{N_e}^s e^{-\beta U} \langle \psi_{0|s}^{n,0} | \prod_{l=1}^n \prod_{k=1}^{N_p} \phi_{kl}^l \phi_{kl}^l, \rangle
\]

where \( U = \frac{1}{n+1} \sum_{l=0}^n \left\{ U_e(X_e^{(l)}, \Delta\beta) + U_p(X_p^{(l)}, \Delta\beta) + U_{ep}(X_p^{(l)}, X_e^{(l)}, \Delta\beta) \right\} \) is the total interaction energy comprised of contributions \( U_e(X_e^{(l)}), U_p(X_p^{(l)}), U_{ep}(X_p^{(l)}, X_e^{(l)}) \) being the sum of pair interactions given by Kelbg potentials. Here \( X^{(l)}_0 \equiv (\kappa_p q^{(0)}_p, \kappa_e q^{(0)}_e), X^{(l)}_l \equiv (X_p^{(l)}, X_e^{(l)}) \) with \( X^{(l)}_a = \kappa_a q^{(0)}_a + \sum_{i=1}^n \eta^{(l)}_a (k \text{ runs from } 1 \text{ to } n) \) and \( X^{(n+1)} = (\kappa_p q^{(n+1)}_p, \kappa_e q^{(n+1)}_e) = X^{(0)} \).

Here we use the familiar Kelbg potential [35, 36]

\[
\Phi_{ab}(x_{ab}; \Delta\beta) = \frac{e_a e_b}{\lambda_{a,b} x_{ab}} \left( 1 - e^{-\pi^2 x_{ab}^2} + \sqrt{\pi} x_{ab} \right) \left\{ 1 - \text{erf}(x_{ab}) \right\},
\]

where \( x_{ab} = \frac{|q_{ka} - q_{tb}|}{\lambda_{a,b}} \), and we introduced the error function, \( \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \, dt \, e^{-t^2} \).

Note that the Kelbg potential is finite at zero distance which is a consequence of quantum effects. The validity of this potential is restricted to temperatures \((1/\Delta\beta)\) substantially higher than the binding energy [37–39] which puts the lower bound on the number of slices \( n \).

Here we use notations

\[
\phi_{kl}^l = \exp[-\pi |x_{kl}^{(l)}|^2], \quad \tilde{\phi}_{kl}^l = \exp[-\pi |\eta_{kl}^{(l)}|^2],
\]

\[
||\psi_{0|s}^{n,0}||_s = \left( e^{-\frac{\pi}{\Delta\lambda^2} \left( |r_k - r_l| + |y_k - y_l| \right)^2} \right)^{N_e - s} \times \left( e^{-\frac{\pi}{\Delta\lambda^2} \left( |r_k - r_l| + |y_k - y_l| \right)^2} \right)^{N_s}.
\]

Notice that the density matrix (4) does not contain an explicit sum over the permutations and, thus, no sum of terms with alternating sign. Instead, the whole exchange problem is contained in the determinant (6) which is a product of exchange matrices of electrons where \( s \) denotes the number of electrons having the same spin projections (for more details, we refer to [40, 41]). This grouping of terms with different signs into the spin determinant is similar to “blocking” algorithms, e.g. [11], and allows to substantially weaken the Fermion sign problem.

### 3. Path integral Monte Carlo procedure

The above formulas have been applied successfully to multi-component dense quantum plasma simulations [26, 28, 30, 42], to the electron-hole plasmas in semiconductors [31, 32] as well as to the quark-gluon plasma [33, 34]. It is, therefore, desirable to retain the same program also for the simulation of jellium where the positive component is treated as a homogeneous static background. This has the advantage that both components are treated consistently, in particular, the background contribution will be automatically adjusted to the chosen particle number (which would not be the case if we would use the known corrections for the case of an infinite system).

To perform the transition to the case of jellium with minimal changes we put the potential energy contributions of the positive charges—the p-p and p-e interactions in the exponent of the high-temperature density matrices—to zero. Thus expression for \( U \) is reduced to \( U = \frac{1}{n+1} \sum_{l=0}^n U_e \left( X_e^{(l)}, \Delta\beta \right) \). At the same time, the interaction terms \( \Psi_{ep} \) and \( \Psi_{pp} \) are retained as they produce the energy contribution of the “background”. With this, the positive charge
component is treated as an ideal gas of given density and temperature with the number positive charges always matching that of the electrons, guaranteeing charge neutrality. With these trivial changes, expressions (3), (4) are well suited for efficient fermionic PIMC simulations of jellium using standard Metropolis Monte Carlo techniques (see, e.g., [5, 9, 10]). In our Monte Carlo scheme we use three different types of moves, where either electronic \( (q_t, e) \) or positive charge coordinates \( (q_p, h) \) or the individual electronic beads \( (n_t^{(k)}) \) are moved until convergence of the calculated values is reached.

4. Simulation results
We now apply the theoretical scheme developed in the preceding sections to polarized jellium. Below, the density of the electrons is characterized by the Brueckner parameter, \( r_s = a/a_B \), defined as the ratio of the mean distance between particles, \( a = \left( \frac{3}{4\pi n_e} \right)^{1/3} \), and the Bohr radius, \( a_B \), where \( n_e \) is electron density. Temperatures will be given in units of the Fermi energy, \( \Theta = k_B T/E_F \).

We now present our fermionic path integral Monte Carlo simulation results for the energy of the uniform electron gas, based on (3), with the simplifications discussed above. We use the same density and temperature interval that was studied in [18]: \( r_s \geq 1 \) and \( \Theta = 0.0625, \ldots, 8 \). Higher densities are not considered since there the sign problem is too severe and the data are not reliable.

For the present simulations we varied, both, the particle number, in the range of \( N_e = N_p = 50 \ldots 100 \), and the number of beads, in the range \( M = 20 \ldots 90 \). Larger bead numbers are presently not feasible for such large systems. This interval of \( N \) and \( M \) has been used to perform an extrapolation to the macroscopic limit. To this end, we first performed an extrapolation \( N \to \infty \), for fixed values of \( M \). These extrapolated data were then used in a second extrapolation with respect to the beads number, \( M \to \infty \). The value of the total error of the described extrapolation including statistical error we estimate as 4-5 percents.

4.1. Polarized electron gas
Figure 1 shows the final results for a polarized electron gas. The left column shows the total energy for four different temperatures, whereas the right columns contain the correlation energy which was calculated as \( E_c = E_{\text{tot}} - E_0 - E_{\text{x, HF}} \), subtracting from the total energy the kinetic energy and the finite temperature Hartree-Fock (mean field plus exchange) energy from [18]. Since \( E_{\text{tot}} \) and \( E_0 + E_{\text{x, HF}} \) are of the same order of magnitude, the remainder (the correlation energy) is very susceptible to different approximations and allows for sensitive comparisons of our results to those from [18].

The curve denoted “\( E_0 \)” shows the (kinetic) energy of an ideal polarized Fermi gas at finite temperature computed from the relevant Fermi integral. The curves “DPIMC \( E_0 \)” show the same result obtained with our fermionic PIMC simulations. For the two highest temperatures, \( \Theta = 8 \) and \( \Theta = 1 \), the results coincide practically for all densities. For \( \Theta = 0.25 \) small deviations are seen at the highest density, \( r_s = 1 \), whereas for \( \Theta = 0.0625 \) deviations are visible up to \( r_s \sim 3 \). This behavior is a very good test for the order of magnitude of the error and for the reliability of simulations.

If interactions are included, the total energy is lower compared to the ideal case. The curves are denoted by “DPIMC” and are compared to the corresponding restricted PIMC data of Brown et al [18] labeled “RPIMC”. Again, the agreement over the entire temperature interval is rather good. An exception is the point \( r_s = 1 \) corresponding to the highest density. For \( \Theta = 0.25 \) our data are substantially lower than RPIMC. Interestingly, for \( \Theta = 0.0625 \) the agreement is significantly better although the accuracy of our results is most likely lower due to the increased sign problem. Also, notice the fermionic (“signful”) PIMC simulations [18] labeled “SFPIMC”
Figure 1. (Color online) Total energy per particle (left column) and correlation energy per particle (right column) for a polarized ideal ($E_0$) and interacting electron gas (PUEG) with temperatures ranging from $\Theta = 8$ to $\Theta = 0.0625$, see text in the graphs. Comparison of restricted PIMC (RPIMC [18]), fermionic PIMC (SFPIMC, open pink circles [18]) and the present DPIMC results. The correlation energy is given by $E_c = E_{tot} - E_0 - E_{c,HF}$ using the Hartree-Fock energy from [18], see main text.)
that are plotted with the open (pink) circles. For low densities we observe good agreement with our data, whereas for \( r_s \leq 4 \) there are significant deviations. At these points the SFPIMC data already carry large error bars and we expect that our results are more accurate.

In contrast to the rather good agreement of the total energies there is a quite large deviation between DPIMC and RPIMC for the correlation energy. Possible reasons for these deviations are a) quantum effects in the interaction of electrons with the uniform background described, in our calculations, by the effective Kelbg pseudopotential, instead of the Coulomb potential. The Kelbg pseudopotential is defined by the logarithm of the high-temperature asymptotic of the quantum two-particle density matrix. The Coulomb potential cannot be obtained in the same way as the classical density matrix of two oppositely charged particles diverges at small interparticle distances. Other sources for deviations are b) the different particle numbers used in DPIMC and RPIMC and c) finite size corrections that are applied to the RPIMC data [18] but not to our results—we instead, performed an extrapolation to the macroscopic limit.

5. Conclusion

In this paper we have presented new direct fermionic path integral Monte Carlo (DPIMC) simulations for the thermodynamic properties of the polarized uniform electron gas over a wide density and temperature range relevant for warm dense matter conditions.

We compared our direct fermionic PIMC simulations with recent restricted PIMC simulations and direct (signful) simulations by Brown et al [18]. First we notice that our simulations carry a much smaller statistical error than the signful results [18], and they are significantly closer to the RPIMC data, at high degeneracy. This is attributed to the improved treatment of exchange in our approach. Second, the comparison to the RPIMC results revealed very good agreement for all densities, \( r_s \geq 1 \), for temperatures above the Fermi energy. For lower temperatures we observe good agreement for moderate densities, \( r_s \geq 4 \). The good agreement, over such a broad range of parameters, between the two independent approaches that involve entirely different approximations is certainly remarkable and considered our main result. Thus, we have mapped out the parameter range where the predictions for the energy of the UEG can be considered reliable.

On the other hand, while the total energies of our DPIMC simulations are in overall good agreement with the RPIMC results [18], we observe significant deviations of the correlation energies. Possible reasons are a) the different treatment of quantum effects in the interaction of electrons with the uniform background, b) the different number of particles in the two simulations and c) finite size corrections which are applied in [18], but not in our results.

Acknowledgments

We acknowledge stimulating discussions with T Schoof, S Groth and T Dornheim (Kiel) and J W Dufty and V Karasiev (University of Florida). The total energy of UEG was calculated in the Joint Institute for High Temperatures RAS under support by the Russian Science Foundation grant No. 14-50-00124, while the correlation energy of UEG was calculated in the Institute for Theoretical Physics and Astrophysics.

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