# Supplementary material for manuscript “Ab initio thermodynamic results for the degenerate electron gas at finite temperature”

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This supplement contains additional information on 1. CPIMC simulations for the polarized electron gas, 2. Thermodynamic Green functions results and 3. the first CPIMC results for the unpolarized (paramagnetic) electron gas.

## 1 First-principle CPIMC simulation results for the spin-polarized electron gas

### 1.1 Energy contributions for the uniform electron gas at finite temperature and high density

Here, we include the configuration path integral Monte Carlo (CPIMC) data for the uniform electron gas used in the figures of the main text. Table 1 contains the total, kinetic and potential energy for 33 fully polarized particles in the canonical ensemble for a broad range of temperatures and densities, together with the total energy of the non-interacting Fermi gas. For $r_s \geq 0.6$, an additional potential $V_\kappa$ restricting the number of kinks was used and the total, kinetic and potential energies were each extrapolated to the unrestricted case, as explained in the main text. Therefore, for these values, the sum of kinetic and potential energy equals the total energy only within the given errors. The errors were constructed to include systematic uncertainties due to the extrapolation. For the ideal Fermi gas, $N_B = 925$ basis function were used. For all other cases the calculations were performed using $N_B = 2109$ basis functions. For $\theta = 1.0$, the basis size used for the ideal Fermi gas was increased to $N_B = 2109$ and for the interacting system to $N_B = 4169$. The basis incompleteness error is less than the statistical error, as explained in the main text. All statistical errors correspond to a $1\sigma$ standard deviation.

In Tab. 2 we present energies per particle for temperatures in the range of $\theta = 2$ to $\theta = 8$ as well as the energy of the ideal Fermi gas. For the CPIMC simulations, $N_B = 5575$, $N_B = 24\,405$, and $N_B = 44\,473$ basis functions have been used for $\theta = 2$, $\theta = 4$, and $\theta = 8$, respectively. An extrapolation with respect to the additional potential $V_\kappa$ was applied to $r_s \geq 2$ for $\theta = 2$ and $r_s = 4$ for $\theta = 4$.

### 1.2 Finite size corrections

To map our data for $N = 33$ particles to the macroscopic limit we use the finite size corrections for the kinetic and potential energy of Drummond *et al.* [1] for the spin polarized case

$$\Delta T(r_s, \beta; N) = \frac{1}{N}\left(\frac{\omega_p}{4} - \frac{5.264}{\pi r_s^2 (2N)^{1/3}} 2^{-2/3}\right) \tag{S1}$$

$$\Delta V(r_s; N) = \frac{\omega_p}{4N}, \tag{S2}$$

where $\beta = 1/k_B T$, and we introduced the plasma frequency $\omega_p = 2\sqrt{\frac{3}{r_s^3}}$ (in units of Rydberg). These formulas were derived for twist averaged boundary conditions [2], so we performed corresponding simulations for two temperatures ($\theta = 0.0625$ and $\theta = 0.5$) and densities from $r_s = 0.01$ to $r_s = 1.0$. As $N = 33$ constitutes a magic number, twist averaging has a small effect for lower densities but becomes more important for $r_s < 1.0$. Formulas (S1, S2) are called “FSC (a)” in the main manuscript and work well for not too high density, although a small deviation from the $e^4$ approximation and the fit of Ref. [9] remains. The deviations grow much faster with density for $\theta = 0.5$, which reflects the fact that these corrections are derived for the ground state.

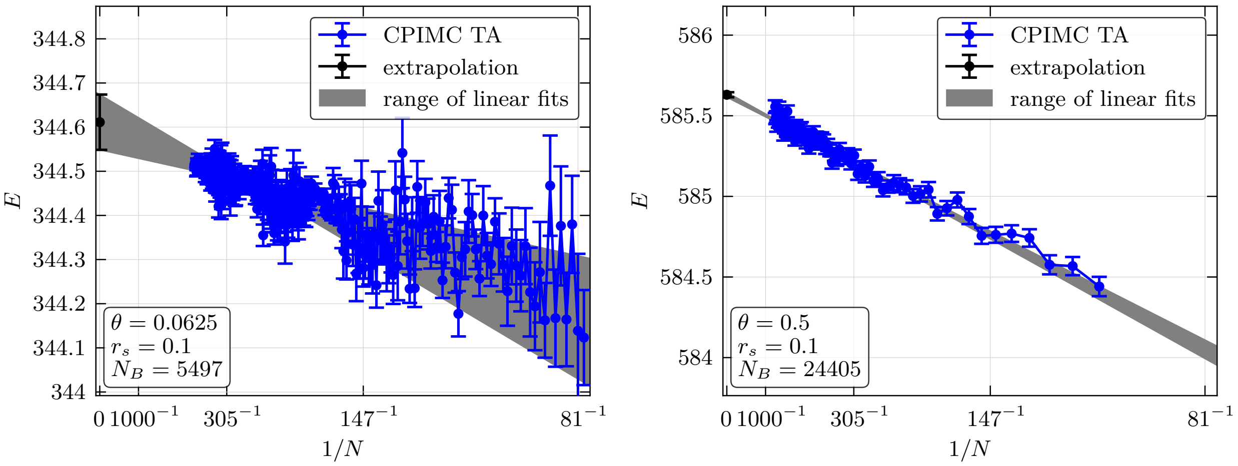

Figure S1: (Color online) Extrapolation to the macroscopic limit. Left, $\theta = 0.0625$; right, $\theta = 0.5$. Blue symbols denote CPIMC total energies per particle for various particle numbers in twist-averaged boundary conditions. The grey area visualizes the range of fits for different choices of the starting- and endpoints. The resulting macroscopic energy is shown in black.

On the path to improve the available finite size corrections for high densities and finite temperatures we also performed twist-averaged CPIMC calculations for up to $N = 800$ particles at $r_s = 0.1$ and two temperatures $\theta = 0.0625$ and $\theta = 0.5$, which allow for a reliable extrapolation of finite-size results to the macroscopic limit. For $r_s = 0.3$, approximate results were obtained for up to $N = 150$ particles by CPIMC calculations which used only even kink numbers. This approach yields reasonable results for low temperatures. In all cases, at least 128 random twist angles have been used. The dependence of the total energy on the particle numbers is in good agreement with a power law of $E(N) \propto N^{-1}$ as used in [1].

Although being greatly reduced by twist-averaging, shell effects are still present in the energy data, introducing a significant dependence on the starting- and endpoint of a fit. For this reason, we fitted the total energy for all possible starting-points in the range $N \in [80, 200]$ ($N \in [100, 200]$) and all possible endpoints in the range $N \in [300, 400]$ ($N \in [600, 800]$) for $r_s = 0.1$ and $\theta = 0.0625$ ($\theta = 0.5$). For $r_s = 0.3$ and $\theta = 0.0625$ particle numbers were chosen between $N \in [80, 100]$ and $N \in [120, 150]$. As it is unclear how to weight the single fits, the final result is simply taken to be the average between the minimal and the maximal extrapolated value with their difference as uncertainty. This is shown in Fig. S1. As for all fits in this work, data points have been weighted relative to their error bar.

Tab. 3 shows the resulting finite-size corrections for $N = 33$ particles, denoted by FSC (b) in the main text. These differ from the analytic formulas Eq. (S1) and Eq. (S2), denoted by FSC (a), by more than 2.3 Ry in the worst case of $\theta = 0.5$, highlighting the importance of improved corrections at high densities and finite temperatures.

## 2 Green functions results for the exchange-correlation energy of the spin-polarized electron gas in Montroll-Ward and $e^4$ approximation

To describe the spin-polarized electron gas in semi-analytical form, we employ the quantum statistical method of thermodynamic Green functions [5, 6]. Its advantage is the ability to describe systems in the thermodynamic limit with arbitrary temperatures including the correct $T=0$ physics, the transition to Boltzmann statistics, and the correct high temperature (Debye-Hückel) law. Using this technique, a perturbation expansion in the interaction strength can be established [6, 7]. Including terms up to the second order, one obtains

$$U_{ee}(T, \alpha_e) = U_e^{\text{id}}(T, \alpha_e) + U_e^{\text{HF}}(T, \alpha_e) + U_{ee}^{\text{MW}}(T, \alpha_e) + U_e^{\text{e}^4\text{n}}(T, \alpha_e) \,. \tag{S3}$$

Here, $\alpha_e = \mu_e / k_B T$ is the activity with the chemical potential $\mu_e$, the temperature $T$, and the Boltzmann constant $k_B$. The terms are the ideal gas law, the Hartree-Fock (HF) quantum exchange term, the direct Montroll-Ward (MW) term, and quantum exchange contributions of the second order ($e^4 n$), respectively. Further, chemical potential and density are related via $n_e \lambda_{DB}^3 = \mathrm{I}_{1/2}(\alpha_e)$, where, $\lambda_{DB} = \sqrt{2\pi\hbar^2 / m_e k_B T}$ is the electron thermal deBroglie wavelength, and $I_\nu$ is the Fermi integral of order $\nu$ [6]. The inversion (transition) from the grand canonical ensemble to the canonical ensemble has already taken place in the golden rule

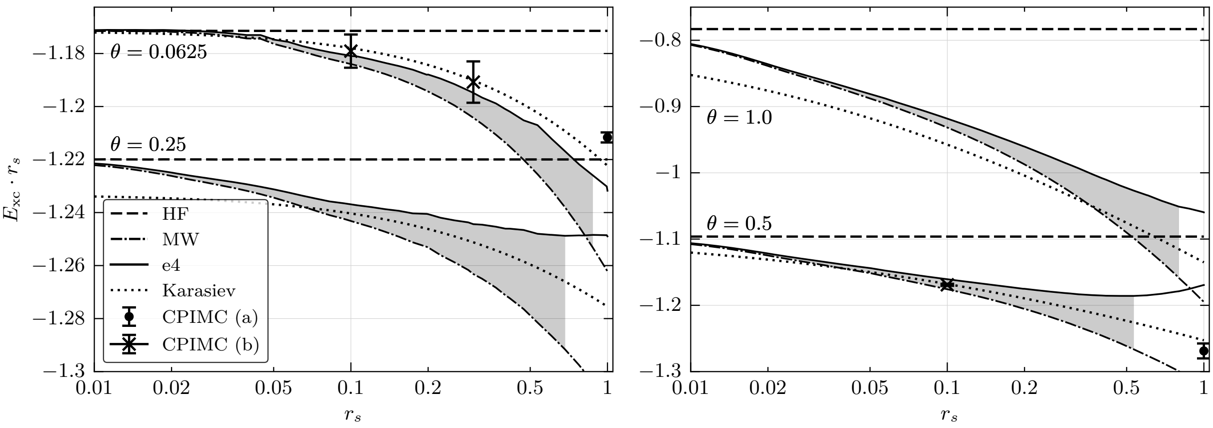

Figure S2: Green functions results for the exchange-correlation energy (times $r_s$) of the polarized uniform electron gas: The Montroll-Ward (MW) and $e^4$ approximation are compared to Hartree-Fock (HF) and the fit of Karasiev *et al.* [9]. The exact result is unknown but expected to be inbetween the $e^4$ and MW curves (cf. shaded area). Due to the weak coupling expansion, the $e^4$ and MW approximations are restricted to small $r_s$ values. The width of the shaded area can be used to judge the validity range of the analytical approximations: we terminate the shaded area when the width exceeds 1% of the mean value of $E_{tot}$. The points with the error bars denote the CPIMC results for $r_s = 1$, applying the finite size correction of Drummond *et al.* [1], Eqs. (S1, S2). The crosses denote the CPIMC extrapolation over $N$, see text and Tab. 3.

approximation, and the resulting additional terms are given below together with the HF, MW and $e^4$ terms. We summarize the results used in the main text.

**1.** The ideal internal energy is given by

$$U_e^{\mathrm{id}}(T, \alpha_e) = \frac{3}{2}\frac{k_B T}{\lambda_{DB}^3} \mathrm{I}_{3/2}(\alpha_e)\,. \tag{S4}$$

**2.** First order exchange contributions are contained in the HF term [6]

$$U_e^{\mathrm{HF}}(T, \alpha_e) = \frac{e^2}{\lambda_{DB}^4} \int\limits_{-\infty}^{\alpha_e} d\alpha\, \mathrm{I}_{-1/2}^2(\alpha) - \frac{3e^2}{2\lambda_{DB}^4} I_{-1/2}(\alpha_e) I_{1/2}(\alpha_e), \tag{S5}$$

where the 2nd term is a direct result of the inversion procedure or can be seen as resulting from the temperature derivative of the free energy.

**3.** The Montroll-Ward contribution to the equation of state can be computed using the dielectric function of the spin-polarized electron gas, $\varepsilon_e(p,\omega) = 1 - V_{ee}(p)\Pi_{ee}(p,\omega)$, with the result [7]

$$p_e^{\mathrm{MW}}(T, \mu_e) \;\; = \;\; \frac{-1}{4\pi^3} \int\limits_0^\infty dp\, p^2\, \mathcal{P}\!\!\int\limits_{\pm 0}^\infty d\omega\, \coth\left(\frac{\hbar\omega}{2k_B T}\right) \left[\arctan \frac{\mathrm{Im}\,\varepsilon_e(p,\omega)}{\mathrm{Re}\,\varepsilon_e(p,\omega)} - \mathrm{Im}\,\varepsilon_e(p,\omega)\right]. \tag{S6}$$

It is consistent with the expansion (S3) to use here the dielectric function in random phase approximation (RPA).

**4.** The normal $e^4$ exchange term for the equation of state, accounting for exchange effects of second order, can be written as an integral over Fermi functions, $f_p = [\exp(\beta p^2/2m_e - \beta\mu_e) + 1]^{-1}$, and Pauli blocking factors, denoted $\bar{f}_p = [1 - f_p]$ [7],

$$p_e^{e^4 n}(T, \mu_e) = \frac{m_e}{2} \int \frac{d\mathbf{p} d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^9} v_{ee}(p) v_{ee}(\mathbf{p} + \mathbf{q}_1 + \mathbf{q}_2) \frac{f_{q_1} f_{q_2} \bar{f}_{\mathbf{q}_1 + \mathbf{p}} \bar{f}_{\mathbf{q}_2 + \mathbf{p}} - f_{\mathbf{q}_1 + \mathbf{p}} f_{\mathbf{q}_2 + \mathbf{p}} \bar{f}_{q_1} \bar{f}_{q_2}}{q_1^2 + q_2^2 - (\mathbf{p} + \mathbf{q}_1)^2 - (\mathbf{p} + \mathbf{q}_2)^2}\,, \tag{S7}$$

where, $v_{ee}$ is the bare electron-electron Coulomb potential.

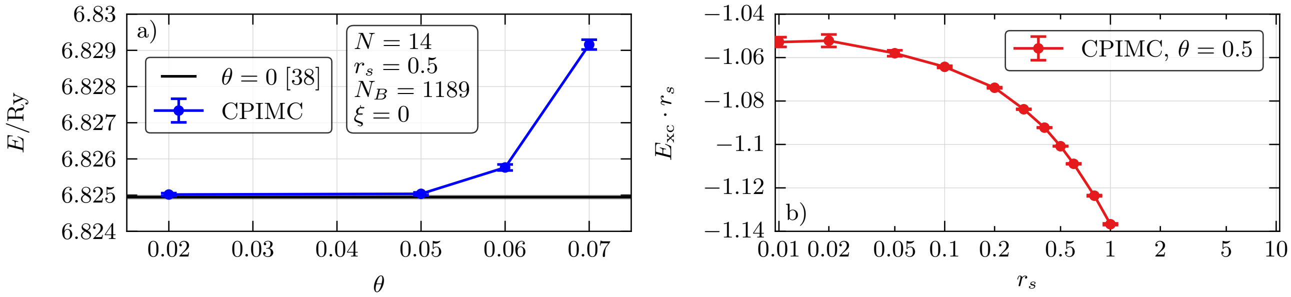

Figure S3: (Color online) CPIMC results for the unpolarized UEG for $N = 14$. **a**: low temperature total energy for $r_s = 0.5$, compared to the ground state data of Ref. [10], horizontal black line, grey area denotes the error bars. **b**: Density dependence of the exchange-correlation energy for $\Theta = 0.5$.

**5.** From the two results for the pressure, Eqs. (S6, S7), the corresponding internal energy contributions follow according to

$$U_e^k(T, \alpha_e) = -p_e^k(T, \alpha_e) + T\frac{\partial}{\partial T} p_e^k(T, \alpha_e), \qquad k = \mathrm{MW}, e^4 n. \tag{S8}$$

The expansion (S3) accounts for direct correlations and dynamic screening, incorporates collective oscillations (plasmons) as well as quantum diffraction and exchange in the electron system. This expression is valid for weakly coupled electrons of arbitrary degeneracy and, in particular, includes the low and high temperature limiting cases of Debye-Hückel as well as Gell-Mann and Brueckner, respectively [7].

In the following, we use the notation "$e^4$ approximation" for the complete expression (S3), whereas "MW" denotes the result (S3) without the last term. Numerical results for the $e^4$ approximation, for two temperatures, are shown in Fig. 5 of the manuscript. Here we present additional data, extending the temperature range to $\Theta = 1$, and we also compare with the Hartree-Fock (HF) and Montroll-Ward (MW) approximations. Figure S2 shows the exchange-correlation energy (times $r_s$) for four temperatures. In all cases, the high-density limit is a horizontal line, approaching the Hartree-Fock approximation. For lower densities approaching $r_s = 1$, MW and $e^4$ start to deviate from each other. Obviously, the series expansion contains sign alternating contributions so we expect that the exact result will be enclosed between the MW- and $e^4$ approximations where $e^4$ yields an upper bound to the exchange-correlation energy. Furthermore, we notice that the agreement between MW- and $e^4$ approximations improves with decreasing temperature.

The data for the total energy in the various analytical approximations are presented in table 1.

## 3 First CPIMC simulation results for the unpolarized electron gas

For the ideal Fermi gas, $N_B = 925$ basis function were used. For all other cases, the calculations were performed using $N_B = 2109$ basis functions. The results for unpolarized electrons with $N = 14$ are shown in Figure S3 and in Table 4. No twist averaging and finite size extrapolation has been performed. The table also contains thermodynamic Green functions results for the macroscopic unpolarized UEG with the same approximations as explained above.

Table 1: **Left part**: CPIMC energies per particle for $N = 33$ polarized electrons: ideal energy, $U_0$, total energy, $E_{\text{tot}}$, kinetic energy, $E_{\text{kin}}$, and potential energy, $E_{\text{pot}}$. **Right part**: total energy per particle of the macroscopic UEG, for different analytical approximations: ideal energy $U_0$ (S4), Hartree-Fock (HF), Eq. (S5), Montroll-Ward (MW), Eqs. (S6, S8) and $e^4$ approximation ($e4$), Eqs. (S7, S8). Energies in units of Ryd.

| | | CPIMC ($N = 33$) | | | | Analytical approximations | | | |
|---|---|---|---|---|---|---|---|---|---|
| $\theta$ | $r_s$ | $U_0$ | $E_{\text{tot}}$ | $E_{\text{kin}}$ | $E_{\text{pot}}$ | $U_0$ | HF | MW | e4 |
| 0.0625 | 0.01 | 35 458.07(4) | 35 336.30(22) | 35 457.65(22) | −121.3612(4) | 35 640.21 | 35 523.06 | 35 523.06 | 35 523.09 |
| | 0.02 | 8864.517(9) | 8803.59(4) | 8864.32(4) | −60.727 38(11) | 8909.727 | 8851.156 | 8851.136 | 8851.168 |
| | 0.05 | 1418.3227(15) | 1393.918(9) | 1418.264(9) | −24.346 28(4) | 1425.608 | 1402.179 | 1402.082 | 1402.114 |
| | 0.10 | 354.5807(4) | 342.358(5) | 354.575(5) | −12.217 61(9) | 356.4021 | 344.6876 | 344.5623 | 344.5928 |
| | 0.20 | 88.645 17(9) | 82.5102(15) | 88.6609(14) | −6.150 73(5) | 89.100 54 | 83.2433 | 83.128 84 | 83.160 94 |
| | 0.30 | 39.397 85(4) | 35.2933(8) | 39.4197(8) | −4.126 41(5) | 39.600 23 | 35.695 41 | 35.586 07 | 35.617 42 |
| | 0.40 | 22.161 292(23) | 19.0740(5) | 22.1871(5) | −3.113 04(5) | 22.275 13 | 19.346 51 | 19.241 05 | 19.272 65 |
| | 0.60 | 9.849 463(10) | 7.7787(14) | 9.8776(11) | −2.097 26(19) | 9.900 058 | 7.947 647 | 7.848 245 | 7.880 411 |
| | 0.80 | 5.540 323(6) | 3.9779(22) | 5.5693(32) | −1.590(4) | 5.568 787 | 4.104 478 | 4.009 63 | 4.040 199 |
| | 1.00 | 3.545 807(4) | 2.2898(15) | 3.5745(34) | −1.2835(34) | 3.564 021 | 2.392 57 | 2.301 711 | 2.332 256 |
| 0.1250 | 0.01 | 37 217.14(6) | 37 092.91(30) | 37 212.95(30) | −120.0438(4) | 37 275.81 | 37 155.89 | 37 155.87 | 37 155.91 |
| | 0.02 | 9304.284(16) | 9242.12(6) | 9302.19(6) | −60.075 62(22) | 9318.611 | 9258.653 | 9258.612 | 9258.648 |
| | 0.05 | 1488.6854(25) | 1463.827(11) | 1487.920(11) | −24.092 91(7) | 1491.032 | 1467.049 | 1466.96 | 1466.995 |
| | 0.10 | 372.1714(6) | 359.715(4) | 371.812(4) | −12.096 87(11) | 372.7581 | 360.7661 | 360.6584 | 360.6927 |
| | 0.20 | 93.042 84(16) | 86.8060(16) | 92.9013(15) | −6.095 27(6) | 93.189 54 | 87.193 55 | 87.098 77 | 87.134 98 |
| | 0.30 | 41.352 37(7) | 37.1833(7) | 41.2755(7) | −4.092 22(6) | 41.417 57 | 37.420 25 | 37.331 13 | 37.366 92 |
| | 0.40 | 23.260 71(4) | 20.1268(6) | 23.2159(6) | −3.089 07(7) | 23.297 38 | 20.299 39 | 20.213 65 | 20.248 08 |
| | 0.60 | 10.338 093(18) | 8.2390(12) | 10.3238(16) | −2.0836(5) | 10.354 39 | 8.355 732 | 8.273 912 | 8.309 463 |
| | 0.80 | 5.815 177(10) | 4.2334(29) | 5.8139(19) | −1.582(8) | 5.824 351 | 4.325 353 | 4.246 401 | 4.281 027 |
| | 1.00 | 3.721 714(6) | 2.450(4) | 3.729(5) | −1.280(9) | 3.727 581 | 2.528 384 | 2.452 161 | 2.487 229 |
| 0.2500 | 0.01 | 43 133.28(8) | 43 005.3(5) | 43 119.7(5) | −114.3657(9) | 43 073.15 | 42 951.16 | 42 950.94 | 42 951 |
| | 0.02 | 10 783.320(19) | 10 719.93(11) | 10 777.18(11) | −57.257 92(34) | 10 767.89 | 10 706.89 | 10 706.58 | 10 706.64 |
| | 0.05 | 1725.3312(30) | 1699.891(18) | 1722.883(18) | −22.992 32(14) | 1722.925 | 1698.526 | 1698.238 | 1698.301 |
| | 0.10 | 431.3328(8) | 418.612(7) | 430.178(7) | −11.566 46(15) | 430.7315 | 418.5319 | 418.2997 | 418.3626 |
| | 0.20 | 107.833 20(19) | 101.4488(15) | 107.2978(15) | −5.849 05(8) | 107.6829 | 101.5831 | 101.417 | 101.4799 |
| | 0.30 | 47.925 87(8) | 43.6591(8) | 47.5981(8) | −3.938 97(7) | 47.859 03 | 43.7925 | 43.648 36 | 43.711 11 |
| | 0.40 | 26.958 30(5) | 23.7508(5) | 26.7321(5) | −2.981 32(7) | 26.920 71 | 23.870 81 | 23.742 75 | 23.805 54 |
| | 0.60 | 11.981 467(21) | 9.8327(12) | 11.8538(14) | −2.0199(7) | 11.964 76 | 9.931 492 | 9.821 115 | 9.884 106 |
| | 0.80 | 6.739 575(12) | 5.1215(21) | 6.662(5) | −1.542(10) | 6.730 183 | 5.205 231 | 5.106 167 | 5.169 354 |
| | 1.00 | 4.313 328(8) | 3.014(4) | 4.262(7) | −1.249(11) | 4.307 315 | 3.087 35 | 2.995 452 | 3.058 339 |

Table 1: *(continued).* **Left part**: CPIMC energies per particle for $N = 33$ polarized electrons: ideal energy, $U_0$, total energy, $E_{\mathrm{tot}}$, kinetic energy, $E_{\mathrm{kin}}$, and potential energy, $E_{\mathrm{pot}}$. **Right part**: total energy per particle of the macroscopic UEG, for different analytical approximations: ideal energy $U_0$ (S4), Hartree-Fock (HF), Eq. (S5), Montroll-Ward (MW), Eqs. (S6, S8) and $e^4$ approximation ($e4$), Eqs. (S7, S8). Energies in units of Ryd.

| | | CPIMC ($N = 33$) | | | | Analytical approximations | | | |
|---|---|---|---|---|---|---|---|---|---|
| $\theta$ | $r_s$ | $U_0$ | $E_{\mathrm{tot}}$ | $E_{\mathrm{kin}}$ | $E_{\mathrm{pot}}$ | $U_0$ | HF | MW | e4 |
| 0.5000 | 0.01 | 59 504.77(16) | 59 380.6(8) | 59 483.0(8) | −102.3978(9) | 59 732.07 | 59 622.44 | 59 621.3 | 59 621.45 |
| | 0.02 | 14 876.19(4) | 14 814.74(18) | 14 866.03(17) | −51.2963(6) | 14 932.47 | 14 877.66 | 14 876.23 | 14 876.38 |
| | 0.05 | 2380.191(6) | 2355.402(25) | 2376.036(25) | −20.634 13(16) | 2389.282 | 2367.357 | 2366.254 | 2366.406 |
| | 0.10 | 595.0477(16) | 582.650(14) | 593.058(14) | −10.408 43(26) | 597.3207 | 586.358 | 585.5635 | 585.7148 |
| | 0.20 | 148.7619(4) | 142.5160(35) | 147.8068(35) | −5.290 79(14) | 149.3301 | 143.8488 | 143.3036 | 143.4549 |
| | 0.30 | 66.116 41(18) | 61.9353(14) | 65.5152(14) | −3.579 92(12) | 66.368 94 | 62.714 72 | 62.277 54 | 62.4288 |
| | 0.40 | 37.190 48(10) | 34.0378(12) | 36.7589(12) | −2.721 07(9) | 37.332 53 | 34.591 87 | 34.218 35 | 34.369 54 |
| | 0.60 | 16.529 10(5) | 14.4093(21) | 16.2673(14) | −1.8577(8) | 16.592 24 | 14.765 13 | 14.466 16 | 14.6174 |
| | 0.80 | 9.297 620(25) | 7.6943(26) | 9.1196(30) | −1.424(4) | 9.333 143 | 7.962 809 | 7.708 448 | 7.8597 |
| | 1.00 | 5.950 477(16) | 4.660(4) | 5.823(6) | −1.162(6) | 5.973 207 | 4.876 941 | 4.652 623 | 4.803 846 |
| 1.0000 | 0.01 | 98 930.9(15) | 98 821.7(26) | 98 908.8(26) | −87.0477(13) | 99 202.77 | 99 124.46 | 99 122.08 | 99 122.22 |
| | 0.02 | 24 732.7(4) | 24 678.7(8) | 24 722.3(8) | −43.6217(6) | 24 799.78 | 24 760.63 | 24 757.84 | 24 757.98 |
| | 0.05 | 3957.24(6) | 3935.63(13) | 3953.20(13) | −17.565 21(30) | 3968.11 | 3952.448 | 3950.353 | 3950.488 |
| | 0.10 | 989.309(15) | 978.392(29) | 987.269(29) | −8.876 69(14) | 992.0277 | 984.1968 | 982.7109 | 982.8453 |
| | 0.20 | 247.327(4) | 241.809(7) | 246.337(7) | −4.527 97(6) | 248.0069 | 244.0914 | 243.0704 | 243.2047 |
| | 0.30 | 109.9232(17) | 106.2045(26) | 109.2790(26) | −3.074 50(5) | 110.2253 | 107.6149 | 106.7979 | 106.9326 |
| | 0.40 | 61.8318(9) | 59.0190(15) | 61.3643(15) | −2.345 234(31) | 62.001 72 | 60.043 98 | 59.347 61 | 59.481 75 |
| | 0.60 | 27.4808(4) | 25.5776(6) | 27.1891(6) | −1.611 536(25) | 27.556 32 | 26.251 16 | 25.697 37 | 25.833 41 |
| | 0.80 | 15.457 95(23) | 14.0102(7) | 15.2531(8) | −1.2429(13) | 15.500 45 | 14.521 58 | 14.051 82 | 14.186 54 |
| | 1.00 | 9.893 09(15) | 8.7214(8) | 9.7379(8) | −1.016 20(22) | 9.920 273 | 9.137 178 | 8.725 332 | 8.860 601 |

Table 2: **Left part**: CPIMC energies per particle for $N = 33$ polarized electrons: total energy, $E_{\text{tot}}$, kinetic energy, $E_{\text{kin}}$, and potential energy, $E_{\text{pot}}$. **Right part**: total ideal energy per particle of the macroscopic UEG $U_0$, Eq. (S4). Energies in units of Ryd.

| | | CPIMC ($N = 33$) | | | Analytical |
|---|---|---|---|---|---|
| $\theta$ | $r_s$ | $E_{\text{tot}}$ | $E_{\text{kin}}$ | $E_{\text{pot}}$ | $U_0$ |
| 2 | 0.01 | 183 285(5) | 183 359(5) | −74.0447(18) | 183 606 |
| | 0.02 | 45 798.6(13) | 45 835.7(13) | −37.1009(8) | 45 901.49 |
| | 0.05 | 7317.02(21) | 7331.95(21) | −14.931 82(29) | 7344.238 |
| | 0.10 | 1824.76(5) | 1832.30(5) | −7.540 91(15) | 1836.06 |
| | 0.20 | 453.875(11) | 457.718(11) | −3.843 04(7) | 459.0149 |
| | 0.30 | 200.673(5) | 203.281(5) | −2.608 21(5) | 204.0066 |
| | 0.40 | 112.2688(29) | 114.2583(29) | −1.989 45(4) | 114.7537 |
| | 0.60 | 49.3465(13) | 50.7147(13) | −1.368 156(27) | 51.001 66 |
| | 0.80 | 27.4380(7) | 28.4931(7) | −1.055 121(21) | 28.688 43 |
| | 1.00 | 17.3488(4) | 18.2145(4) | −0.865 710(24) | 18.3606 |
| | 2.00 | 4.0557(7) | 4.5340(4) | −0.4779(4) | 4.590 149 |
| | 3.00 | 1.662(9) | 2.0104(33) | −0.353(15) | 2.040 066 |
| 4 | 0.01 | 356 381(29) | 356 446(29) | −65.4691(22) | 356 620.9 |
| | 0.02 | 89 058(6) | 89 091(6) | −32.7831(12) | 89 155.23 |
| | 0.05 | 14 242.9(11) | 14 256.1(11) | −13.1747(5) | 14 264.84 |
| | 0.10 | 3556.76(24) | 3563.40(24) | −6.638 01(24) | 3566.209 |
| | 0.20 | 887.28(5) | 890.65(5) | −3.367 82(10) | 891.5523 |
| | 0.30 | 393.479(21) | 395.756(21) | −2.277 09(7) | 396.2455 |
| | 0.40 | 220.847(10) | 222.578(10) | −1.731 12(5) | 222.8881 |
| | 0.60 | 97.685(5) | 98.869(5) | −1.184 028(28) | 99.061 37 |
| | 0.80 | 54.6867(25) | 55.5962(25) | −0.909 488(22) | 55.722 02 |
| | 1.00 | 34.8168(22) | 35.5607(22) | −0.743 913(29) | 35.662 09 |
| | 2.00 | 8.4690(4) | 8.8769(4) | −0.407 964(16) | 8.915 523 |
| | 4.00 | 1.9826(9) | 2.2149(6) | −0.2318(6) | 2.228 881 |
| 8 | 1.00 | 69.840(33) | 70.501(33) | −0.660 83(11) | 70.572 06 |

Table 3: Total energies per particle for $N = 33$ polarized electrons in twist-averaged boundary conditions, extrapolated results for the corresponding macroscopic system, analytic FSC (a) from Eqs. (S1, S2), FSC (b) obtained from CPIMC extrapolation, and analytic approximations, see Eqs. (S6, S8) and Eqs. (S7, S8). Energies per particle in units of Ryd.

| $\theta$ | $r_s$ | $E_{\text{tot}}$ ($N = 33$) | $E_{\text{tot}}$ ($N \to \infty$) | FSC (a) | FSC (b) | MW | $e^4$ |
|---|---|---|---|---|---|---|---|
| 0.0625 | 0.1 | 344.354(28) | 344.61(7) | 0.868 265 | 0.26(8) | 344.5623 | 344.5928 |
| | 0.3 | 35.5033(28) | 35.631(26) | 0.231 478 | 0.128(26) | 35.586 07 | 35.617 42 |
| 0.5 | 0.1 | 582.39(7) | 585.630(16) | 0.868 265 | 3.24(7) | 585.5635 | 585.7148 |

Table 4: **Left part**: CPIMC energies per particle for $N = 14$ unpolarized electrons: ideal energy, $U_0$, total energy, $E_{\mathrm{tot}}$, kinetic energy, $E_{\mathrm{kin}}$, and potential energy, $E_{\mathrm{pot}}$. **Right part**: total energy per particle of the macroscopic UEG, for different analytical approximations: ideal energy $U_0$ (S4), Hartree-Fock (HF), Eq. (S5), Montroll-Ward (MW), Eqs. (S6, S8) and $e^4$ approximation ($e4$), Eqs. (S7, S8). Energies in units of Ryd.

| | | CPIMC ($N = 14$) | | | | Analytical approximations | | | |
|---|---|---|---|---|---|---|---|---|---|
| $\theta$ | $r_s$ | $U_0$ | $E_{\mathrm{tot}}$ | $E_{\mathrm{kin}}$ | $E_{\mathrm{pot}}$ | $U_0$ | HF | MW | e4 |
| 0.5 | 0.01 | 37 754.74(15) | 37 649.45(16) | 37 747.23(16) | −97.779(4) | 37 569.14 | 37 482.26 | 37 480.82 | 37 480.97 |
| | 0.02 | 9438.68(4) | 9386.07(14) | 9435.18(14) | −49.1027(7) | 9391.883 | 9348.443 | 9346.659 | 9346.81 |
| | 0.05 | 1510.189(6) | 1489.029(26) | 1508.803(26) | −19.774 46(29) | 1502.658 | 1485.283 | 1483.893 | 1484.044 |
| | 0.10 | 377.5473(15) | 366.905(5) | 376.900(5) | −9.995 01(13) | 375.6689 | 366.9809 | 366.013 | 366.1639 |
| | 0.20 | 94.3868(4) | 89.0174(13) | 94.1160(13) | −5.098 68(8) | 93.917 07 | 89.573 11 | 88.913 97 | 89.065 38 |
| | 0.30 | 41.949 71(17) | 38.3371(6) | 41.7986(6) | −3.461 52(6) | 41.741 07 | 38.845 09 | 38.319 85 | 38.4714 |
| | 0.40 | 23.596 71(10) | 20.866 06(31) | 23.505 55(31) | −2.639 48(4) | 23.4793 | 21.307 32 | 20.861 43 | 21.013 51 |
| | 0.50 | 15.101 89(6) | 12.900 26(18) | 15.044 19(17) | −2.143 93(5) | 15.026 79 | 13.2892 | 12.896 86 | 13.048 51 |
| | 0.60 | 10.487 43(4) | 8.639 24(33) | 10.451 21(26) | −1.811 82(16) | 10.435 26 | 8.987 27 | 8.633 526 | 8.790 687 |
| | 0.80 | 5.899 177(24) | 4.4947(4) | 5.887 89(29) | −1.393 05(28) | 5.869 834 | 4.783 843 | 4.484 474 | 4.636 478 |
| | 1.00 | 3.775 474(16) | 2.6387(4) | 3.7782(15) | −1.1396(17) | 3.756 692 | 2.8879 | 2.621 94 | 2.774 52 |

# References

[1] N. D. Drummond, R. J. Needs, A. Sorouri, and W. M. C. Foulkes, *Finite-size errors in continuum quantum Monte Carlo calculations*, Phys. Rev. B **78**, 125106 (2008).

[2] C. Lin, F. H. Zong, and D. M. Ceperley, *Twist-averaged boundary conditions in continuum quantum Monte Carlo algorithms*, Phys. Rev. E **64**, 016702 (2001).

[3] For $r_s \gtrsim 1$ Brown *et al.* [4] proposed a temperature correction to the ground state formula (S1, S2) which, however, does not yield reasonable results for $r_s \leq 1$.

[4] E.W. Brown, B. K. Clark, J. L. DuBois, and D. M. Ceperley, *Path-Integral Monte Carlo Simulation of the Warm Dense Homogeneous Electron Gas*, Phys. Rev. Lett. **110**, 146405 (2013).

[5] W.-D. Kraeft, W. Kremp, W. Ebeling, G. Röpke, *Quantum Statistics of Charged Particle Systems* Akademie Verlag (Berlin), (1986).

[6] D. Kremp, M. Schlanges, W.-D. Kraeft, *Quantum Statistics of Nonideal Plasmas* Springer (Berlin), (2005).

[7] J. Vorberger, M. Schlanges, W.-D. Kraeft, *Equation of state for weakly coupled quantum plasmas*, Phys. Rev. E **69**, 046407 (2004).

[8] M. Gell-Mann, K.A. Brueckner, *Correlation Energy of an Electron Gas at High Density*, Phys. Rev. **106**, 364 (1957).

[9] V.V. Karasiev, T. Sjostrom, J. Dufty, and S. B. Trickey *Accurate Homogeneous Electron Gas Exchange-Correlation Free Energy for Local Spin-Density Calculations*, Phys. Rev. Lett. **112**, 076403 (2014) and Supplementary Material.

[10] J.J. Shepherd, G.H. Booth, and A. Alavi, *Investigation of the full configuration interaction quantum Monte Carlo method using homogeneous electron gas models*, J. Chem. Phys. **136**, 244101 (2012).