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Equation of state and correlation energy of dense plasmas

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Abstract

In this paper, the method of thermodynamic Green's functions is applied to investigate thermodynamic properties of dense weakly coupled plasmas. First, we present results for the equation of state for fully ionized hydrogen and compare our results with path integral Monte Carlo simulation data. Densities and temperatures are considered where correlations as well as Fermi statistics have to be taken into account. Then, the correlation energy and the mean value of the kinetic energy of dense plasmas are considered. Usually one finds that the kinetic energy is larger than that of an ideal system due to the interaction. However, in agreement with results from quantum simulations, we found, for certain densities and temperatures, a lowering of the kinetic energy.

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1. Introduction

The current progress in experimental investigations of dense non-ideal plasmas has led to an increasing interest in the theoretical description of matter under extreme conditions relevant for inertially confined fusion and astrophysics. Here, recent equation of state (EOS) measurements in liquid deuterium are intensely discussed [1–3]. The physical interpretation and modelling of the experimental findings require a basic understanding of the influence of quantum and correlation effects on the properties of strongly coupled plasmas. In this connection, the developments in the field of *ab initio* numerical simulations have become of increasing importance [4–9]. On the other hand, rigorous methods of quantum statistical theory are available for obtaining accurate analytical results in the limiting cases of weakly and highly degenerate quantum systems [10–12]. This provides the possibility to compare simulation data with analytical results in density–temperature regions where agreement has to be expected.

The aim of this paper is to investigate the thermodynamic properties of the weakly coupled hydrogen plasma and the quantum electron gas using the method of thermodynamic Green's

functions. Densities and temperatures are considered where correlations as well as Fermi statistics have to be taken into account. Results for the EOS are compared to data recently obtained from path integral Monte Carlo (PIMC) simulations. Furthermore, correlation effects on the mean value of the kinetic energy are investigated. Usually one expects in quantum systems that the kinetic energy is larger than that of an ideal system due to the interaction in the system. However, in agreement with quantum HNC calculations [13] and recent PIMC simulations [14, 15], we found, for certain densities and temperatures, a lowering of the mean value of kinetic energy in dense plasmas.

In this way, the quantum statistical calculations presented in this paper are a contribution for closing the gap between analytical approaches and numerical simulations.

2. Thermodynamic properties of dense weakly coupled plasmas

2.1. EOS of fully ionized hydrogen

An appropriate starting point to determine the EOS of dense plasmas is to calculate the pressure directly using the charging formula in the grand canonical ensemble

$$(p - p_{\text{id}})\Omega = - \int_0^1 \frac{d\lambda}{\lambda} \langle \lambda V \rangle_\lambda \quad (1)$$

with Ω being the volume. The mean value of the potential energy can be expressed in terms of the two-particle Green's function, i.e.

$$\langle \lambda V \rangle_\lambda = \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 \lambda V(\mathbf{r}_1 - \mathbf{r}_2) G_2(12, 1^{++}2^+) |_{t_2=1_1^+}. \quad (2)$$

We used, e.g., $1 = \mathbf{r}_1, t_1$ where the spin variables were dropped for simplicity. For details concerning the method of Green's function techniques in quantum statistical theory, we refer to [11]. In the following we will consider weakly coupled plasmas so that bound states can be neglected and it is sufficient to calculate the EOS in Montroll–Ward approximation including the Hartree–Fock (HF) and Montroll–Ward (MW) diagrams (exchange-correlation; xc). For the pressure, the following expression can be achieved [16]:

$$\begin{aligned} p(\beta\mu_c^0) = & \sum_a \frac{2\sigma_a + 1}{\beta\Lambda_a^3} I_{3/2}(\beta\mu_a^0) \\ & + \sum_a \frac{(2\sigma_a + 1)e_a^2}{\Lambda_a^4} \mathcal{I}_{\text{HF}}(\beta\mu_a^0) - \sum_a \frac{(2\sigma_a + 1)e_a^2}{\Lambda_a^4} I_{-1/2}(\beta\mu_a^0) I_{1/2}(\beta\mu_a^0) \\ & + p_{\text{MW}}(\beta\mu_c^0) - \sum_a k_B T \frac{I_{1/2}(\beta\mu_a^0)}{I_{-1/2}(\beta\mu_a^0)} \frac{\partial}{\partial \mu_a} p_{\text{MW}}(\beta\mu_a) \Big|_{\beta\mu_a^0} \end{aligned} \quad (3)$$

where $I_\nu(\alpha)$ denote the Fermi integrals, μ_a^0 is the ideal chemical potential and $\Lambda_a = (2\pi\hbar^2/m_a k_B T)^{1/2}$ is the thermal wavelength of species a .

To obtain the pressure as a function of the density, one has to use the relation $n_a(\beta\mu_a^0) = (2s_a + 1)I_{1/2}(\beta\mu_a^0)/\Lambda_a^3$. The first term on the rhs of equation (3) is the pressure of the ideal quantum plasma, and the contributions given in the second line follow from the HF exchange diagram. Here, $\mathcal{I}_{\text{HF}}(\alpha)$ is the Hartree–Fock integral given in equation (11) [17]. In the third line, we have the contributions to the MW pressure with

$$p_{\text{MW}}(\alpha) = \int_0^\infty \frac{d\mathbf{q}}{(2\pi)^3} \mathcal{P} \int_0^\infty \frac{d\omega}{2\pi} \coth\left(\frac{\beta\omega}{2}\right) \left[\arctan \frac{\text{Im } \varepsilon(\mathbf{q}, \omega)}{\text{Re } \varepsilon(\mathbf{q}, \omega)} - \text{Im } \varepsilon(\mathbf{q}, \omega) \right]. \quad (4)$$

Here, the dielectric function $\varepsilon(\mathbf{q}, \omega)$ is taken in random phase approximation (see, e.g., [11]). It should be noted that the level of approximation given by equation (3) is appropriate to

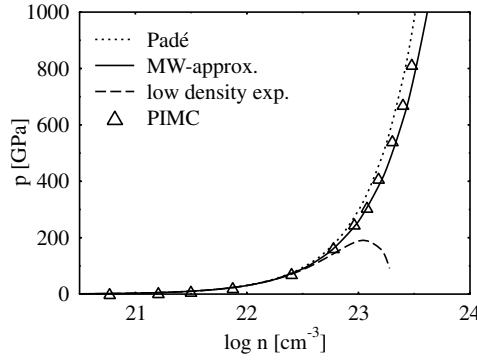


Figure 1. Pressure as a function of the density for a hydrogen plasma at $T = 125\,000$ K: Montroll–Ward approximation (3), low density expansion [12], Padé approximation [18] and results from PIMC calculations [19].

determine the EOS for weakly coupled plasmas at any degeneracy. Consequently, it covers the range of the classical low density limit as well as the highly degenerate quantum plasma. In this way, reliable and accurate results for the EOS can be obtained which provides the possibility to compare our results with simulation data obtained for densities and temperatures where agreement has to be expected.

In figure 1, results for the EOS of a fully ionized hydrogen plasma are shown as a function of the density for a temperature $T = 125\,000$ K. In particular the pressure obtained in different approximations is compared to PIMC simulation data. There is good agreement between all approaches at low densities. Deviations occur at higher densities where Fermi statistics and correlation effects become important. The simulations lead to slightly higher pressure values than the xc approximation calculated from equation (3) but they are lower than the results from the Padé formula given in [18].

2.2. Correlation effects on the mean kinetic energy

In the following we will focus on special features concerning the influence of quantum and correlation effects on the internal energy of dense plasmas. The latter consists of the sum of the mean values of kinetic and potential energies, respectively,

$$U = \langle H \rangle = \langle K \rangle + \langle V \rangle. \quad (5)$$

The mean value of the potential energy was given already by expression (2) in terms of the two-particle Green's function. The mean kinetic energy can be calculated from

$$\langle K \rangle = \sum_a \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{p^2}{2m_a} f_a(\mathbf{p}) \quad (6)$$

with $f_a(\mathbf{p})$ being the Wigner distribution function of species a . For interacting quantum systems, $\langle K \rangle$ includes correlations as the momentum distribution deviates from that of the ideal gas. Therefore, the internal energy can be written as

$$U = \langle K \rangle^{\text{id}} + U^{\text{corr}} = \langle K \rangle^{\text{id}} + \langle K \rangle^{\text{corr}} + \langle V \rangle \quad (7)$$

with $\langle K \rangle^{\text{id}} + \langle K \rangle^{\text{corr}} = \langle K \rangle$ and U^{corr} being the total correlation energy.

For classical contributions, we have $\langle K \rangle = \langle K \rangle^{\text{id}}$ whereas for quantum systems one usually expects an increase in the mean value of the kinetic energy $\langle K \rangle$ as a result of the interaction between the particles. This is observed, e.g., in the limit $T = 0$. However,

at finite temperatures, also the opposite case is possible, i.e., a lowering of the kinetic energy as compared to that of the non-interacting system. Such a behaviour was found some years ago using a quantum HNC approach [13] and recently in PIMC simulations [14, 15].

Here, we will discuss this problem in the framework of Green's function techniques [20]. In particular, high enough temperatures are considered so that bound states can be neglected, and it is sufficient to calculate the thermodynamic functions in the Montroll–Ward (xc) approximation as was done in the previous section. We determine the free energy which, in the canonical ensemble, is given by

$$F - F^{\text{id}} = \int_0^1 \frac{d\lambda}{\lambda} \langle V \rangle_{|\lambda} \quad (8)$$

according to the *golden rule* of statistical mechanics. As we are interested in the behaviour of the ratios $U^{\text{corr}}/\langle V \rangle$ and $\langle K \rangle/\langle K \rangle^{\text{id}}$, the correlation energy U^{corr} is calculated from

$$U = F - T \frac{\partial F}{\partial T} \quad (9)$$

and $\langle K \rangle$ from equation (7).

Let us first give an estimate concerning the lowering of the kinetic energy using the low density expansion of the thermodynamic quantities up to the order n^2 [10, 12]. Accounting for the xc terms we get

$$\frac{U_{\text{xc}}}{\langle V \rangle_{\text{xc}}} = 1 - \frac{\sqrt{\pi}}{16} \kappa \lambda + \pi \frac{n \lambda^3}{\kappa \lambda}. \quad (10)$$

This ratio is larger than unity if the condition $k_B T > 1 \text{ Ryd}$ is fulfilled. In this way, the density expansion (10) indicates the possibility of a lowering of the mean kinetic energy for high temperatures.

Now we will perform a numerical evaluation of the xc contributions. The mean value of the Hartree–Fock potential energy

$$\frac{1}{\Omega} \langle V \rangle_{\text{HF}} = -\frac{2e^2}{\Lambda^4} \mathcal{I}_{\text{HF}}(\alpha) \quad \mathcal{I}_{\text{HF}}(\alpha) = \int_{-\infty}^{\alpha} I_{-1/2}^2(y) dy \quad (11)$$

does not change the sign for any degeneracy. For this contribution, the correlation part of the free energy follows to be $F_{\text{HF}} = \langle V \rangle_{\text{HF}}$, with $\langle V \rangle_{\text{HF}}$ given by (11). Then, using (9), we get for the correlation energy related to the potential energy

$$\frac{U_{\text{HF}}}{\langle V \rangle_{\text{HF}}} = -1 + \frac{3}{2} \frac{I_{-1/2}(\alpha) I_{1/2}(\alpha)}{\mathcal{I}_{\text{HF}}(\alpha)}. \quad (12)$$

This ratio (12) is shown in figure 2 as a function of the density for a temperature $T = 1 \times 10^6 \text{ K}$ (short-dashed line). It gives the value 2 in the low density limit and approaches unity for high degeneracy. It turns out that, in the Hartree–Fock approximation at finite temperatures, there is always $\langle K \rangle < \langle K \rangle^{\text{id}}$.

Now we turn to the numerical calculation of the Montroll–Ward contribution. For the mean value of the potential energy, we use the expression

$$\langle V \rangle_{\text{MW}} = \Omega \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d\mathbf{p}}{(2\pi)^3} n_B(\omega) [\text{Im} \varepsilon^{-1}(\mathbf{p}, \omega) + \text{Im} \varepsilon(\mathbf{p}, \omega)]. \quad (13)$$

The corresponding contribution to the internal energy follows from equation (9) with the free energy determined by equation (8). Numerical results for the ratio $U^{\text{corr}}/\langle V \rangle$ are presented in figure 2. The solid line shows the results for the ratio $U^{\text{corr}}/\langle V \rangle$ in the xc approximation. In fact, there is a range where the ratio is larger than unity. In this range, the HF contribution plays the dominant role. For comparison, the results following from the asymptotic

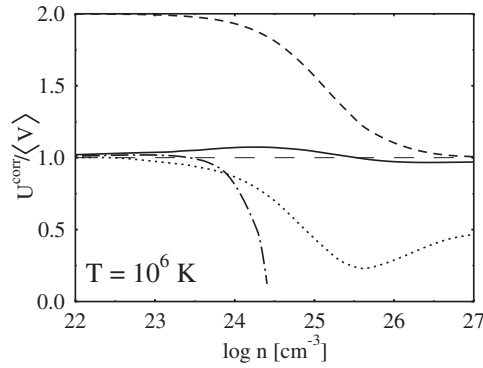


Figure 2. Ratio of correlation and potential energies for an electron gas versus density at temperature $T = 1 \times 10^6$ K in different approximations: HF (short-dashed), MW (dotted), HF+MW (solid) and low density expansion (10) (dash-dotted).

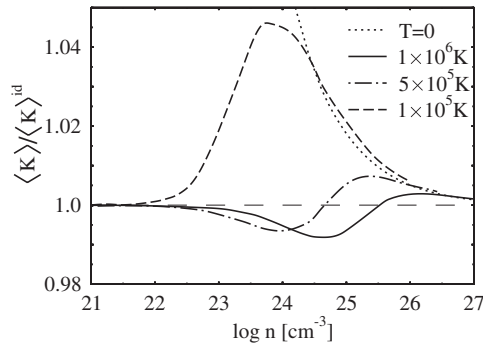


Figure 3. Ratio of the mean kinetic energy of an interacting electron gas and that of the ideal system versus density. The curves present the results in the xc approximation for different temperatures.

expansion (10) are also presented. The resulting behaviour of the mean value of the kinetic energy can be seen in figure 3. Here, the ratio $\langle K \rangle / \langle K \rangle^{\text{id}}$ is shown in the xc approximation as a function of the density for different temperatures. At the lowest temperature given ($T = 1 \times 10^5$ K), the ratio is larger than unity in the density range shown. However, at higher temperatures, there is a range with a well developed lowering of the mean kinetic energy which corresponds to the case where the ratio $U^{\text{corr}} / \langle V \rangle$ exceeds unity as shown in figure 2. Therefore, at finite temperatures, we find $\langle K \rangle / \langle K \rangle^{\text{id}} \geq 1$. The result obtained in this paper follows from the inclusion of quantum and correlation effects which was realized here in exchange-correlation approximation. It clearly shows regions, where the kinetic energy of an interacting system is smaller than that of a free system. This is impossible at $T = 0$. Indeed, at higher densities the ratio $\langle K \rangle / \langle K \rangle^{\text{id}}$ is larger than unity and it merges for any temperature into the curve for the limiting case $T = 0$.

Our calculations confirm results found by HNC [13] and PIMC calculations [14, 19] at finite temperatures. We also made calculations for hydrogen plasmas using the xc approximation. The results are similar to those of the electron gas.

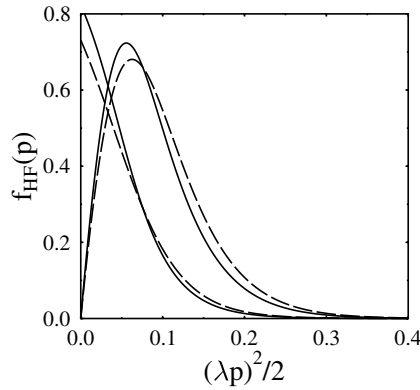


Figure 4. Single-particle distribution function of an electron gas as a function of $(\lambda p)^2/2$: ideal system (dashed) and HF model (solid line). The distribution function multiplied by $(\lambda p)^2/2$ is also included. The parameters are $\lambda/a_B = 5$, $\beta\mu = 1$ (free) and $\beta\mu = 0.530\,02$ (HF).

2.3. Single-particle distribution function

In the preceding sections, we determined thermodynamic functions starting with a certain approximation for the mean value of the potential energy. Thermodynamic properties may also be expressed in terms of single-particle properties. According to (6), the mean kinetic energy is determined by the Wigner function which is defined as

$$f_a(\mathbf{p}) = \sum_{s_a} \int \frac{d\omega}{2\pi} f_a(\omega) A_a(\mathbf{p}, \omega) \quad (14)$$

with $f_a(\omega)$ being the Fermi function and $A_a(\mathbf{p}, \omega)$ being the single-particle spectral function [11]. Therefore, it is also of special interest to study how the interaction influences the behaviour of the single-particle distribution. It is known that there might be algebraic tails in contrast to the simple shape of Fermi functions for ideal systems. In particular, we want to find out how the effect of the lowering of the mean kinetic energy is reflected in the behaviour of the single-particle distribution function $f_a(\mathbf{p})$.

The simplest example is the Hartree–Fock case where we have

$$A_a(\mathbf{p}, \omega) = 2\pi \delta \left(\omega - \frac{p^2}{2m_a} - \Sigma_a^{\text{HF}}(\mathbf{p}) \right). \quad (15)$$

The (real) self-energy takes the form (V_{aa} —Coulomb potential)

$$\Sigma_a^{\text{HF}}(\mathbf{p}) = - \int \frac{d\mathbf{q}}{(2\pi)^3} V_{aa}(\mathbf{p} - \mathbf{q}) f_a(E(\mathbf{q})) \quad E(\mathbf{q}) = \frac{q^2}{2m_a} + \Sigma_a^{\text{HF}}. \quad (16)$$

To go beyond the HF approximation is a very difficult problem (see, e.g., [21–23]). In this case, the self-energy has an imaginary part leading to a broadening of the spectral function and thus to a damping of the single-particle motion. For systems with the possibility of the formation of bound states, it is necessary to use the (screened) ladder (T -matrix) approximation [11, 24]. As an example, we consider the Hartree–Fock model and determine the single-particle distribution function $f_{\text{HF}}(p) = f_a\left(\frac{p^2}{2m_a} + \Sigma_a^{\text{HF}}(p)\right)$ self-consistently with (16) for the electron gas [22, 20]. The chemical potential was chosen to get equal densities for the case of free particles (ideal system) and for the HF approximation. We found, for the physical system given, that the distribution function in the HF model is shifted to lower momenta as compared to the ideal gas. This can be seen in figure 4. Consequently, in the HF model, the correlation

energy is larger than the mean potential energy, in agreement with our results discussed in the previous section.

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