

**Kinetic and correlation energies and distribution functions of dense plasmas**

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The mean value of the kinetic energy of a quantum plasma is investigated in Hartree-Fock and Montroll-Ward approximations using the method of thermodynamic Green's functions. Usually, one finds the kinetic energy to be larger than that of an ideal plasma due to the interaction between the particles in the system. However, also the opposite case is possible, i.e., a decrease of the kinetic energy compared to that of the ideal gas. This special correlation effect is found for temperatures of about  $10^6$  K and densities between  $10^{21}$  and  $10^{26}$   $\text{cm}^{-3}$ . Here, the single-particle distribution function is shifted towards smaller momenta, and the binary distribution is changed.

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**I. INTRODUCTION AND BASIC EQUATIONS**

The progress in experimental investigations of nonideal plasmas leads to a further increasing interest in the theoretical description of matter under extreme conditions relevant for inertially confined fusion and astrophysics. There are experiments by Bastea *et al.* [1] which deal with the question of metal-insulator transitions. The equation of state measurements by Knudson *et al.* [2] in liquid deuterium show good agreement with Path Integral Monte-Carlo calculations by Militzer and Ceperley [3,4] and Militzer *et al.* [5] and do not agree with the former hugoniots found by DaSilva *et al.* [6]. Recent investigations of electron-ion systems at very low temperatures have initiated molecular dynamic simulations [7,8] and stimulated the formulation of thermodynamic formulas valid for any degeneracy especially also for the heavier species. Here, the role of the initial correlations and the question of possibilities for cooling of degenerate quantum systems is of current interest [9–13]. The physical interpretation and modeling of the recent experimental findings require a basic understanding of the influence of quantum and correlation effects on the properties of strongly coupled plasmas. Thus, *ab initio* numerical simulations have become of increasing importance covering a wide range of density and temperature [3–5,14–16]. On the other hand, rigorous methods of quantum statistical theory are available to get reliable and accurate analytical results in the limiting cases of weakly and highly degenerate quantum systems [18,19]. This provides the possibility of comparing simulation data with analytical results in density-temperature regions where agreement has to be expected. In this connection, we also mention the attempts by Juranek *et al.* [20] and Knaup *et al.* [21]. In the following, we determine the influence of correlation effects on the different contributions to the internal energy of dense plasmas, and we investigate single particle and radial distribution functions.

The internal energy corresponds to the expectation value of the Hamiltonian, and consists, consequently, of the sum of

the mean values of kinetic and potential energies, respectively,

$$U = \langle H \rangle = \langle K \rangle + \langle V \rangle. \quad (1)$$

The mean value of the potential energy is given in terms of the two-particle Green's function

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

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 Ref. [19]. The mean value of the kinetic energy can be calculated from

$$\langle K \rangle = \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{p^2}{2m} f(\mathbf{p}), \quad (3)$$

with  $f(\mathbf{p})$  being the Wigner distribution function. It is well known that for quantum systems the mean value of the kinetic energy includes correlation effects as the momentum distribution deviates from that of the ideal gas due to the interaction in the system. Therefore, it is necessary to distinguish between the mean value of the potential energy and the total correlation energy  $U^{\text{corr}}$ . Instead of Eq. (1), we can write

$$U = \langle K \rangle^{\text{id}} + \langle K \rangle^{\text{corr}} + \langle V \rangle = \langle K \rangle^{\text{id}} + U^{\text{corr}}, \quad (4)$$

with  $\langle K \rangle^{\text{id}} + \langle K \rangle^{\text{corr}} = \langle K \rangle$ . For classical contributions, we have  $U^{\text{corr}} = \langle V \rangle$ , in quantum systems, however, one usually expects an increase of the mean value of the kinetic energy  $\langle K \rangle$  as a result of the interaction between the particles. Such a behavior follows, e.g., in the limiting case at  $T=0$ . However, at finite temperatures also the opposite case is possible, i.e., a decrease of the kinetic energy as compared to the noninteracting system. Such a behavior was found in path integral Monte Carlo Simulations by Pierloni *et al.* [15] for fully ionized hydrogen, some years ago by Pokrant [17] using quantum-HNC, and recently by Militzer and Pollock [22]

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for the electron gas model at finite temperatures. They found that in some range of density and temperature the kinetic energy  $\langle K \rangle$  is smaller than the kinetic energy  $\langle K \rangle^{\text{id}}$  of the ideal system, i.e., the correlation energy  $|U^{\text{corr}}|$  is larger than the mean potential energy  $|\langle V \rangle|$ .

The goal of this paper is to discuss the question how correlations change the mean value of the kinetic energy of dense plasmas using Green's function techniques. In particular, as a numerical example, an electron gas (OCP) is considered with number density  $n$  and temperature  $T$ . We start our discussion under the assumption that we have some approximate analytical expression for the mean value of the potential energy  $\langle V \rangle$  according to Eq. (2). There, the potential energy is given in terms of the chemical potential, and the equation of state (EOS) is achieved after elimination of the chemical potential by an inversion procedure. We do not want to go into details here; see Ref. [19]. According to the *golden rule* of statistical mechanics, we adopt the point of view that the correlation part of pressure times volume as a function of the chemical potential is equal to the negative correlation part of the free energy as a function of the density which is, in the canonical ensemble, determined by

$$F - F^{\text{id}} = \int_0^1 \frac{d\lambda}{\lambda} \langle V \rangle |_{\lambda}. \quad (5)$$

Having the free energy, we may determine the internal energy (1) according to

$$U = F - T \frac{\partial F}{\partial T}. \quad (6)$$

We are interested in the differences in the interaction contributions. Therefore, we have to determine  $F^{\text{corr}} = F - F^{\text{id}}$  given by Eq. (5) and then to calculate  $U^{\text{corr}}$  from Eq. (6) and  $\langle K \rangle^{\text{corr}}$  from Eq. (4). On the level of the Hartree-Fock and Montroll-Ward approximation [exchange correlation, (xc)], we discuss the behavior of the ratios  $U^{\text{corr}}/\langle V \rangle$  and  $\langle K \rangle/\langle K \rangle^{\text{id}}$ , respectively. Further, we consider the radial distribution function as well as the single-particle distribution function of the electron gas. It will be shown that, in the framework of the quantum statistical approach used here, there is a possibility for a decrease of the kinetic energy at certain densities and temperatures due to the interaction in the system.

## II. SERIES EXPANSIONS FOR $\langle V \rangle$ , $F^{\text{corr}}$ , AND $U^{\text{corr}}$

Starting from the low-density (weakly degenerate) situation, we assume the mean value of the potential energy to be given in terms of a power series with respect to the coupling strength  $e^2$ . For increasing density, any of the contributions has, in addition, to be multiplied by powers of the degeneracy parameter  $n\Lambda^3$  with  $n$  being the density and  $\Lambda = h/\sqrt{2\pi m k_B T}$  the thermal de Broglie wavelength. This is due to the fact that any of the distribution functions accounts for degeneracy; in perturbation theories the Fermi distributions shows up as a power series of the degeneracy parameter.

Another effect which has to be accounted for is screening. This leads to the fact that contributions of the mean value of the potential energy contain powers of  $\kappa\lambda$ , where  $\kappa^{-1} = \sqrt{k_B T / (4\pi n e^2)}$  is the Debye screening length, and  $\lambda = \hbar/\sqrt{2\mu k_B T}$  is the thermal wavelength, ( $\mu$ -reduced mass).

According to Eq. (5) we have to perform a charging procedure with respect to the coupling strength ( $e^2$ ), and after (6) a differentiation with respect to the temperature has to be performed. Thus we may adopt the following general expression for a typical term of the mean value of the potential energy where we show explicitly the powers of  $e^2$  and  $T$ . We have then (omitting logarithmic terms)

$$\langle V \rangle_{\nu\sigma\tau} = V_{\nu\sigma\tau} = C_{\nu\sigma\tau} \frac{1}{T^{1/2}} \left( \frac{e^2}{T^{1/2}} \right)^\nu \frac{1}{T^{3\sigma/2}} \frac{(e^2)^{\tau/2}}{T^\tau}. \quad (7)$$

The general term of Eq. (7) is of density order  $n^{2+\sigma+\tau/2}$ , where  $\sigma=0,1,\dots$ ,  $\tau=-1,0,1,\dots$ . This term may be written as

$$V_{\nu\sigma\tau} = C_{\nu\sigma\tau} \frac{(e^2)^{\nu+\tau/2}}{T^{-1/2+\nu/2+3\sigma/2+\tau}}. \quad (8)$$

The corresponding correlation part of the free energy follows from Eq. (5), and gives

$$F_{\nu\sigma\tau}^{\text{corr}} = \frac{1}{\nu+\tau/2} V_{\nu\sigma\tau}. \quad (9)$$

The correlation energy can be calculated from Eq. (4), and reads

$$U_{\nu\sigma\tau}^{\text{corr}} = \frac{1}{\nu+\tau/2} (3/2+\nu/2+3\sigma/2+\tau) V_{\nu\sigma\tau}. \quad (10)$$

There is no difference between  $U_{\nu\sigma\tau}^{\text{corr}}$  and  $V_{\nu\sigma\tau}$ , if the prefactor in Eq. (10) is unity, leading to

$$\nu - \tau = 3(\sigma + 1).$$

This condition is fulfilled for the Debye limiting law where  $\nu=2$ ,  $\tau=-1$ , and  $\sigma=0$ . The Debye contribution is a classical term. The condition is also fulfilled for the (classical)  $e^6$  term, where  $\nu=3$  and  $\sigma=\tau=0$ . Further terms, such as ladder type terms are known; they correspond to  $\nu=4,5,6,\dots$ ,  $\sigma=\tau=0$ . Moreover, there are logarithmic terms and some more lower order diagrams which will not be discussed here [19,23,24]. Only some of the coefficients  $C_{\nu\sigma\tau}$  are known explicitly [18]. The task is to set up certain expression for  $\langle V \rangle$  and discuss, e.g., the ratio  $U^{\text{corr}}/\langle V \rangle$ .

## III. HARTREE-FOCK AND MONTROLL-WARD APPROXIMATIONS

We consider high enough temperatures so that bound states do not form and it is sufficient to consider only the Hartree-Fock (HF) and the Montroll-Ward (MW) contributions to the thermodynamic functions. Our numerical discus-

sion below refers only to the electron gas. The Hartree contribution is assumed to be compensated against the positive background in which the OCP is embedded. The first candidate which produces a lowering of the kinetic energy as compared to the ideal situation is the Hartree-Fock contribution. In the low-density region, the Hartree-Fock term is of the order  $e^2$  (see below for the self-consistent HF model). From Eq. (7) it follows for  $\nu=1$  and for  $\sigma=\tau=0$ ,

$$U_{100}^{\text{corr}} = 2V_{100} = 2\langle V \rangle_{\text{HF}} = -2 \frac{k_B T \kappa^3}{8\pi} \pi \frac{n\lambda^3}{\kappa\lambda}. \quad (11)$$

The total energy then reads

$$U = \langle K \rangle_{\text{HF}} + \langle V \rangle_{\text{HF}}, \quad \langle K \rangle_{\text{HF}} = \langle K \rangle^{\text{id}} + \langle V \rangle_{\text{HF}}.$$

As  $\langle V \rangle_{\text{HF}}$  is negative, the mean value of the kinetic energy  $\langle K \rangle_{\text{HF}}$  in a Hartree-Fock system is smaller than the ideal kinetic energy  $\langle K \rangle^{\text{id}}$ . In order to get a more reliable estimate concerning the possibility for a lowering of the mean kinetic energy of a dense nonideal plasma we have to go beyond the Hartree-Fock contribution. Let us first restrict ourselves to high temperatures. Then it is sufficient to take into account only the so-called exchange-correlation (xc)-contributions, i.e.,  $\langle V \rangle = \langle V \rangle_{\text{xc}}$  and  $U^{\text{corr}} = U_{\text{xc}}$ . In the nondegenerate case, the potential energy for xc for electrons can be written up to the order  $n^2$  (in a two component system, the heavier particles are nondegenerate, too, if the electrons are; the heavier particles may still be nondegenerate, if the electrons are degenerate). Accounting for the HF and MW terms we get (only  $e^2$  exchange)

$$\langle V \rangle_{\text{xc}} = -\frac{k_B T \kappa^3}{8\pi} \left( 1 - \frac{\sqrt{\pi}}{4} \kappa\lambda + \pi \frac{n\lambda^3}{\kappa\lambda} \right). \quad (12)$$

The correlation energy follows then to be

$$U_{\text{xc}} = -\frac{k_B T \kappa^3}{8\pi} \left( 1 - \frac{5\sqrt{\pi}}{16} \kappa\lambda + \frac{2\pi n\lambda^3}{\kappa\lambda} \right), \quad (13)$$

and the ratio

$$\frac{U_{\text{xc}}}{\langle V \rangle_{\text{xc}}} = 1 - \frac{\sqrt{\pi}}{16} \kappa\lambda + \pi \frac{n\lambda^3}{\kappa\lambda} \quad (14)$$

is larger than unity, if

$$\frac{4\hbar}{e^2 \sqrt{\pi m_e}} (k_B T)^2 > (k_B T)^{3/2}. \quad (15)$$

The inequality (15) is fulfilled, if  $k_B T > 1$  Ry. In this way, the density expansion (14) indicates the possibility of a lowering of the mean kinetic energy for high temperatures both for the electron gas and a multicomponent system.

Now we will perform a numerical evaluation of the exchange-correlation contributions at any degeneracy including the HF and MW terms.

The mean value of the Hartree-Fock potential energy (being equal to the correlation part of the free energy) does not change the sign for any degeneracy. One finds that the tem-

perature derivative being done numerically does not change the situation found in the nondegenerate case (Cf. [25]). We start from the expression [26]

$$\frac{1}{\mathcal{V}} \langle V \rangle_{\text{HF}} = -\frac{2e^2}{\Lambda^4} \mathcal{I}_{\text{HF}}(\alpha), \quad \mathcal{I}_{\text{HF}}(\alpha) = \int_{-\infty}^{\alpha} I_{-1/2}^2(y) dy, \quad (16)$$

and have to consider

$$\frac{\partial}{\partial T} \frac{1}{\Lambda^4} \mathcal{I}_{\text{HF}}(\alpha) = \frac{2}{T\Lambda^4} \mathcal{I}_{\text{HF}}(\alpha) + \frac{1}{\Lambda^4} \frac{\partial \mathcal{I}_{\text{HF}}}{\partial T}, \quad (17)$$

where  $\mathcal{V}$  denotes the volume.  $I_\nu$  are Fermi integrals, and the connection between  $\alpha$  and  $T$  will be determined as follows. We apply  $I_{1/2}(\alpha) = [n\Lambda^3/(2s+1)]$  and get

$$\frac{\partial \mathcal{I}_{\text{HF}}}{\partial T} = \frac{\partial \mathcal{I}_{\text{HF}}}{\partial \alpha} \frac{\partial \alpha}{\partial T} = -\frac{3}{2T} I_{-1/2} I_{1/2}.$$

The limiting behavior for  $\mathcal{I}_{\text{HF}}$  is [see Ref. [19], Eqs. (6.37) and (6.38)] at low degeneracy,

$$\mathcal{I}_{\text{HF}}(\alpha) = \frac{1}{2} \exp(2\alpha) - \frac{2^{1/2}}{3} \exp(3\alpha), \quad (18)$$

and at high degeneracy,

$$\mathcal{I}_{\text{HF}}(\alpha) = \frac{2}{\pi} \alpha^2 - \frac{\pi}{3} \ln \alpha + 0.504. \quad (19)$$

The correlation part of the free energy follows to be (golden rule)  $F_{\text{HF}} = \langle V \rangle_{\text{HF}}$ , with  $\langle V \rangle_{\text{HF}}$  given by Eq. (16). Then, using Eqs. (2) and (3), we get for the correlation energy related to the potential energy

$$\frac{U_{\text{HF}}}{\langle V \rangle_{\text{HF}}} = -1 + \frac{3}{2} \frac{I_{-1/2}(\alpha) I_{1/2}(\alpha)}{\mathcal{I}_{\text{HF}}(\alpha)}. \quad (20)$$

This ratio (20) is shown in Fig. 1 as a function of the density for a temperature  $T = 5 \times 10^5$  K (dotted line).

The limiting behavior in the weakly degenerate case can be seen to be in agreement with the corresponding formulas (11), the ratio (20) gives the value 2. For high degeneracy, the curve approaches unity; at  $T=0$  there is no difference between  $U^{\text{corr}}$  and  $F^{\text{corr}}$ . It turns out that, in Hartree-Fock approximation at finite temperatures, there is always  $\langle K \rangle < \langle K \rangle^{\text{id}}$ , as the potential energy is negative.

Now we turn to the numerical calculation of the (generalized) Montroll-Ward contribution for the quantum electron gas. For this we need the contribution corresponding to the internal energy (6) which is determined by the free energy and its derivative with respect to the temperature. Furthermore the mean value of the potential energy (2) has to be calculated. For the numerical evaluation we start from the following expression for the Montroll-Ward contribution to the mean value of the potential energy

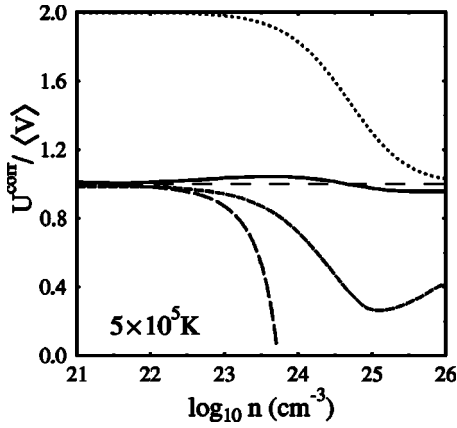


FIG. 1. Ratio of correlation and potential energies for an electron gas versus density at the temperature  $T = 5 \times 10^5$  K in different approximations: HF (dotted), MW (short dashed), and HF+MW (solid); low-density expansion (14) (long dashed).

$$\langle V \rangle_{\text{MW}} = \mathcal{V} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d\mathbf{p}}{(2\pi)^3} n_B(\omega) \times [\text{Im } \varepsilon^{-1}(\mathbf{p}, \omega) + \text{Im } \varepsilon(\mathbf{p}, \omega)]. \quad (21)$$

The dielectric function  $\varepsilon(\mathbf{p}, \omega)$  is taken in random phase approximation (see, e.g., Ref. [19]) and reads

$$\varepsilon(\mathbf{p}, \omega) = 1 + \frac{8\pi e^2}{p^2} \int \frac{d\mathbf{p}'}{(2\pi)^3} \frac{f(\mathbf{p}'+\mathbf{p}) - f(\mathbf{p}')}{\omega + i\epsilon + E(\mathbf{p}') - E(\mathbf{p}'+\mathbf{p})}. \quad (22)$$

The Bose-type function  $n_B(\omega) + 1/2$  is an odd function of  $\omega$ , so are the functions  $\text{Im } \varepsilon^{-1}$  and  $\text{Im } \varepsilon$ . In order to avoid problems with the plasmon peak, and taking into account that both  $\text{Im } \varepsilon$  and  $\text{Im } \varepsilon^{-1}$  fulfill sum rules, however, with opposite signs, e.g.,

$$\int_{-\infty}^{+\infty} d\omega \omega \text{Im } \varepsilon^{-1}(\mathbf{p}, \omega) = -\pi \omega_{pl}^2,$$

we rewrite the integrand of Eq. (21) for an integral between 0 and  $\infty$  only,

$$\langle V \rangle_{\text{MW}} = \mathcal{V} \int_0^{\infty} \frac{d\omega}{2\pi} \int \frac{d\mathbf{p}}{(2\pi)^3} \text{Im } \varepsilon(\mathbf{p}, \omega) \left[ 1 - \frac{1}{|\varepsilon(\mathbf{p}, \omega)|^2} \right] \times \left[ 2n_B(\omega) \left( 1 - \frac{\omega n_B(\Omega)}{\Omega n_B(\omega)} \right) + \left( 1 - \frac{\omega}{\Omega} \right) \right]. \quad (23)$$

In practical calculations, dimensionless frequencies and momenta are used. The frequency  $\Omega$  is the maximum position of  $\text{Im } \varepsilon^{-1}$  which is close to the plasma frequency and is, for small momenta,  $\Omega = 1 + 3[\hbar p / (2m_e \hbar \omega_{pl})^{1/2}]^2$ . At  $\omega = \Omega$ , the integrand is zero and does no longer represent a problem. The integration over  $\omega$  in Eq. (21) may be carried out using Eq. (23). The remaining momentum dependence is shown below in Fig. 5; this is just the momentum representation of

the radial distribution function. For the determination of the MW contribution to the correlation energy

$$U_{\text{MW}} = F_{\text{MW}} - T \frac{\partial F_{\text{MW}}}{\partial T},$$

we need still the free energy which is given by

$$F_{\text{MW}} = \mathcal{V} \int \frac{d\mathbf{p}}{(2\pi)^3} \int_0^{\infty} \frac{d\omega}{2\pi} \coth\left(\frac{\beta\omega}{2}\right) \times \left\{ \arctan \frac{\text{Im } \varepsilon(\mathbf{p}, \omega)}{\text{Re } \varepsilon(\mathbf{p}, \omega)} - \text{Im } \varepsilon(\mathbf{p}, \omega) \right\}. \quad (24)$$

The ratio  $U_{\text{MW}}/\langle V \rangle_{\text{MW}}$  is presented in Fig. 1 for the temperature  $T = 5 \times 10^5$  K. At low densities it tends to unity which is the result for the classical (Debye) limiting law. With increasing density, first there is a decreasing behavior followed by an increase at very high densities. It should be noticed that, at  $T=0$ , the free energy is equal to the internal one. Here we have  $U_{\text{MW}}/\langle V \rangle_{\text{MW}} \rightarrow 0.5$  in the high-density limit. The solid line in Fig. 1 shows the numerical results for the ratio  $U^{\text{corr}}/\langle V \rangle$  including the HF and MW contributions, i.e.,  $U^{\text{corr}} = U_{\text{HF}} + U_{\text{MW}}$  and  $\langle V \rangle = \langle V \rangle_{\text{HF}} + \langle V \rangle_{\text{MW}}$ . We see that there is a range where the ratio is larger than unity. There the Hartree-Fock contribution plays the dominating role. This is the case, e.g., for such densities, where in the MW contribution, the deviations from the (Debye) limiting law are small, and where the HF term is big enough. For comparison, the results following from the asymptotic expansion (14) are presented, too. As expected, the curves coincide at low densities.

The resulting behavior for the mean kinetic energy can be seen in Fig. 2 for different temperatures.

Here, the ratio  $\langle K \rangle / \langle K \rangle^{\text{id}}$  is shown in different approximations as a function of the density. As discussed above, there is always  $\langle K \rangle < \langle K \rangle^{\text{id}}$  in the Hartree-Fock approximation (dotted lines). The situation changes if the MW-contribution is included (solid lines). Now, at the lower temperature  $T = 1 \times 10^5$  K, the ratio is larger than unity in the density range shown. However, at the 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 Fig. 1. This fact is, in general, of interest in connection with recent efforts to investigate possibilities of *cooling* of nonideal plasmas. The result obtained in this paper follows from the inclusion of quantum and correlation effects which was realized here in exchange-correlation approximation including the Hartree-Fock and the Montroll-Ward contributions. Thus, one of our main results is the ratio  $\langle K \rangle / \langle K \rangle^{\text{id}} \geq 1$  at finite temperatures, presented in Fig. 2. It clearly shows regions, where the kinetic energy of an interacting system is smaller than the kinetic energy 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 into the curve for the limiting case  $T=0$ .

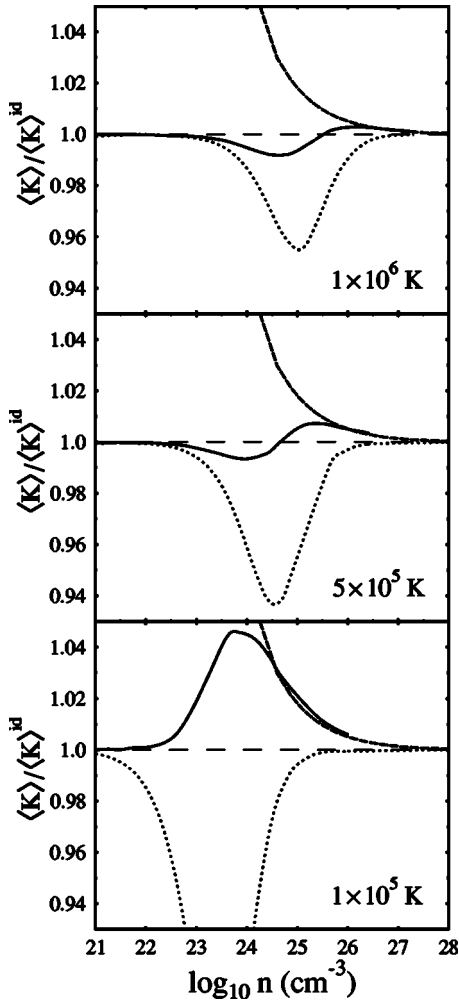


FIG. 2. Ratio of the mean kinetic energy of the interacting electron gas and that of the ideal system versus density for different temperatures. Different approximations are considered: HF (dotted), HF+MW (solid), HF+MW at  $T=0$  (dashed).

A more precise presentation of the behavior just discussed is shown in Fig. 3 for a temperature  $T=1 \times 10^6$  K. Additionally, the results following from the low-density expansions (12) and (13) are given there.

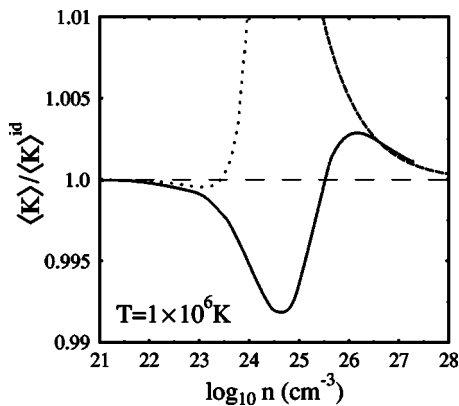


FIG. 3. Ratio of the mean kinetic energies versus density for the temperature  $T=1 \times 10^6$  K: HF+MW approximation (solid), low-density expansion (dotted), HF+MW in the limit  $T=0$  (dashed).

#### IV. SINGLE PARTICLE AND RADIAL DISTRIBUTION FUNCTIONS

So far we determined thermodynamic functions starting with certain approximation for the mean value of the potential energy. Thermodynamic functions may also be determined from the density as a function of the chemical potential, if the single-particle spectral function  $A_a(\mathbf{p}, \omega)$  is known. We may write

$$n_a(\mu_a, T) = \sum_{s_a} \int \frac{d\omega}{2\pi} \frac{d\mathbf{p}}{(2\pi)^3} f_a(\omega) A_a(\mathbf{p}, \omega), \quad (25)$$

with  $f_a(\omega)$  being the Fermi function. Further thermodynamic functions may be expressed in terms of single-particle properties. For example, the mean value of the total energy reads [27]

$$U = \langle H \rangle = \sum_a \sum_{s_a} \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{d\omega}{2\pi} \frac{\omega + \frac{p^2}{2m}}{2} A_a(\mathbf{p}, \omega) f_a(\omega),$$

and the mean value of the potential energy is

$$\langle V \rangle = \sum_a \sum_{s_a} \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{d\omega}{2\pi} \frac{\omega - \frac{p^2}{2m}}{2} A_a(\mathbf{p}, \omega) f_a(\omega).$$

The main ingredient of Eq. (25) is the single-particle distribution function (Wigner function)  $f_a(\mathbf{p})$ , which is defined as

$$f_a(\mathbf{p}) = \sum_{s_a} \int \frac{d\omega}{2\pi} f_a(\omega) A_a(\mathbf{p}, \omega). \quad (26)$$

According to Eq. (3) the Wigner function determines the behavior of the kinetic energy, which was investigated in the preceding sections. Therefore, it is also of special interest to study how the interaction influences the behavior of the single-particle distribution. It is known that there might be algebraic tails in contrast to the simple shape of Fermi functions  $f_{id}$  for ideal systems. We want to find out how the effect of the lowering of the mean kinetic energy is reflected in the behavior of the single-particle distribution function  $f_a(\mathbf{p})$ .

The self energy  $\Sigma_a$  is the key quantity entering the spectral function. The latter has the general shape

$$A_a(\mathbf{p}, \omega) = \frac{2 \text{Im} \Sigma_a(\mathbf{p}, \omega)}{\left[ \omega - \frac{p^2}{2m_a} - \text{Re} \Sigma_a(\mathbf{p}, \omega) \right]^2 + [\text{Im} \Sigma_a(\mathbf{p}, \omega)]^2}, \quad (27)$$

where the imaginary part of the self-energy,  $\text{Im} \Sigma_a(\mathbf{p}, \omega)$ , is related to the damping of the single-particle states, and the real part  $\text{Re} \Sigma_a(\mathbf{p}, \omega)$  determines the energy shift.

The simplest example is the Hartree-Fock case. Then we have  $\text{Im} \Sigma_a = 0$ , and

$$A_a(\mathbf{p}, \omega) = 2\pi \delta\left(\omega - \frac{p^2}{2m_a} - \Sigma_a^{\text{HF}}(\mathbf{p})\right). \quad (28)$$

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

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

$$E(\mathbf{q}) = \frac{q^2}{2m_a} + \Sigma_a^{\text{HF}}. \quad (29)$$

The nondegenerate formula for the Hartree-Fock self-energy reads

$$\Sigma_a^{\text{HF}}(p) = - \frac{2e_a^2}{2s_a+1} n_a \Lambda_{a1}^2 F_1\left(1, \frac{3}{2}; -\frac{\hbar^2 p^2}{2m_a k_B T}\right). \quad (30)$$

with  ${}_1F_1$  being the confluent hypergeometric function. In the HF case, the Fermi distribution function for the electrons is given by

$$f_{\text{HF}}(p) = f_a\left(\frac{p^2}{2m} + \Sigma_a^{\text{HF}}(p)\right) \quad (31)$$

The next order (MW contribution) is very difficult (see, e.g., Refs. [29–31]). 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. The real and imaginary parts of the MW self-energy to be used in Eq. (27) read in first-order iteration

$$\text{Im } \Sigma_a^{\text{MW}}(\mathbf{p}, \omega) = -2\pi\hbar \int \frac{d\mathbf{p}'}{(2\pi)^3} \int \frac{d\omega'}{2\pi} V_{aa}(\mathbf{p}')$$

$$\times (1 - f_a(\mathbf{p} + \mathbf{p}') + n_B(\omega')) \text{Im } \varepsilon^{-1}(\mathbf{p}', \omega' + i\epsilon) \delta\left(\hbar(\omega - \omega') - \frac{\hbar^2}{2m_a}(\mathbf{p} + \mathbf{p}')^2\right) \quad (32)$$

and

$$\text{Re } \Sigma_a^{\text{MW}}(\mathbf{p}, \omega) = -2\hbar \mathcal{P} \int \frac{d\mathbf{p}'}{(2\pi)^3} \int \frac{d\omega'}{2\pi} V_{aa}(\mathbf{p}') \frac{1 - f_a(\mathbf{p} + \mathbf{p}') + n_B(\omega')}{\hbar(\omega - \omega') - \frac{\hbar^2}{2m_a}(\mathbf{p} + \mathbf{p}')^2} \text{Im } \varepsilon^{-1}(\mathbf{p}', \omega' + i\epsilon). \quad (33)$$

For more general spectral functions one has to go beyond the HF and MW approximations of the self-energy. For systems with the possibility of the formation of bound states it is necessary to use the (screened) ladder ( $T$ -matrix) approximation.

If  $\text{Im } \Sigma_a(\mathbf{p}, \omega)$  is small, the spectral function (27) may be expanded with respect to the latter quantity. The result would be the *extended quasiparticle approximation*, consisting of a  $\delta$ -distribution part and a widened part. For a two-component plasma, the latter accounts also for bound states [19,28].

As an example, we solve the Eqs. (31) and (29) self-consistently for the electron gas, i.e., with HF quasiparticles (Hartree-Fock model [30,31]). We find that the Hartree-Fock self energy leads to higher momenta in the distribution, if the chemical potential  $\beta\mu$  is unchanged. However, we want to compare expressions for the kinetic energy at a given density (25) for a free and for an interacting system. To determine the density  $n$  of the electron gas, the momentum integration and spin summation over the distribution function have to be performed,

$$n = \int \frac{d\mathbf{p}}{(2\pi)^3} f(\mathbf{p}). \quad (34)$$

For  $\beta\mu$  fixed, Eq. (34) gives different results for  $f_{\text{id}}$  and  $f_{\text{HF}}$ . Therefore we choose  $\beta\mu$  in the density integrals such that the density according to Eq. (34) is equal. For the thermal

wavelength  $\lambda/a_B = 5$ , our numerical result is as follows: The value  $\beta\mu = 5$  for free particles corresponds to  $\beta\mu = 3.9473$  for  $f_{\text{HF}}$ , while  $\beta\mu = 1$  for  $f_{\text{id}}$  leads to  $\beta\mu = 0.53002$  for  $f_{\text{HF}}$ . Consequently, for the physical system given, the distribution functions in the HF model are shifted to lower momenta as compared to the ideal system. This can be seen in Fig. 4 where in addition, the functions  $p^2 f_{\text{HF}}(p)$  are shown.

Once the distribution function is known, the mean value of the kinetic energy has to be determined according to Eq. (3). For the first situation mentioned above, the kinetic energy of the HF system is 96% of that of the ideal situation, in the second one we get 91%.

This means, in the HF model, the correlation energy is larger than the mean potential energy in agreement with our results discussed in the preceding section.

Finally, we will analyze the consequences of quantum and correlation effects on the radial distribution function of the electron gas. The radial distribution function  $g(\mathbf{p})$  (as a function of the momentum) may be calculated from the mean value of the potential energy discussed above as a functional derivative with respect to the interaction potential. The radial distribution  $g(\mathbf{r})$  is then determined by the Fourier transformation. We have the identity

$$\frac{1}{V} \langle V \rangle = \frac{n^2}{2} \int \frac{d\mathbf{p}}{(2\pi)^3} V(\mathbf{p}) g(\mathbf{p}) = \frac{n^2}{2} \int d\mathbf{r} V(\mathbf{r}) g(\mathbf{r}). \quad (35)$$

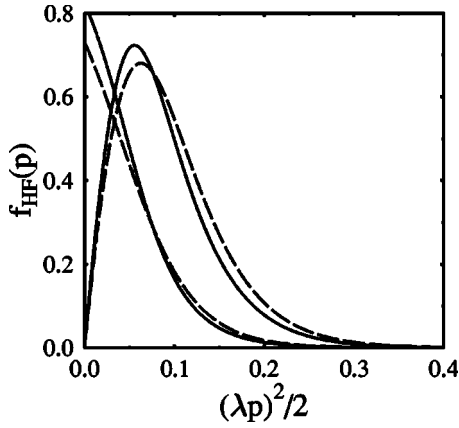


FIG. 4. Single-particle distribution function of an electron gas as a function of  $(\lambda p)^2/2$ : Ideal system (dashed) and HF model (solid line). There is included also the distribution function multiplied by  $(\lambda p)^2/2$ . The parameters are  $\lambda/a_B=5$ ,  $\beta\mu=1$  (free), and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

The first nontrivial term is the contribution corresponding to the ideal exchange of two particles (HF contribution of the two-particle Green's function). In momentum representation, we have

$$g_{\text{HF}}(p) = \frac{2}{n^2} \frac{m_e k_B T}{(2\pi)^2 p} \int_0^\infty \frac{q dq}{\exp\left(\frac{1}{2}\lambda^2 q^2 - \beta\mu\right) + 1} \times \ln \left[ \frac{1 + \exp[-1/2\lambda^2(q+p)^2 + \beta\mu]}{1 + \exp[-1/2\lambda^2(q-p)^2 + \beta\mu]} \right]. \quad (36)$$

Both Eq. (36) and its Fourier transform are given in Fig. 5. The latter, in the low-density case including the direct ideal term, reads [32]

$$g_{\text{id}}(r) = 1 - \frac{1}{2} \exp\left(-\frac{r^2}{\lambda^2}\right). \quad (37)$$

The next order of the momentum representation of the radial distribution function follows from Eq. (21) omitting the momentum integration and the Coulomb potential included in the dielectric functions,

$$g_{\text{MW}}(\mathbf{p}) = \frac{2}{n^2} \int_{-\infty}^\infty \frac{d\omega}{2\pi} \frac{n_B(\omega)}{V(p)} [\text{Im} \varepsilon^{-1}(\mathbf{p}, \omega) + \text{Im} \varepsilon(\mathbf{p}, \omega)]. \quad (38)$$

After a Fourier transformation of Eq. (38), the radial distribution is found in position space. It is also shown in Fig. 5 together with the momentum representation. An electron gas is considered with temperature  $k_B T = 1$  Ry and number density  $n = 1.35 \times 10^{23} \text{ cm}^{-3}$ . As expected, for not too high densities, there is excellent agreement between the Montroll-Ward approximation and the Debye distribution at larger distances. This can be seen in Fig. 6 where the radial distribution function of the quantum electron gas,

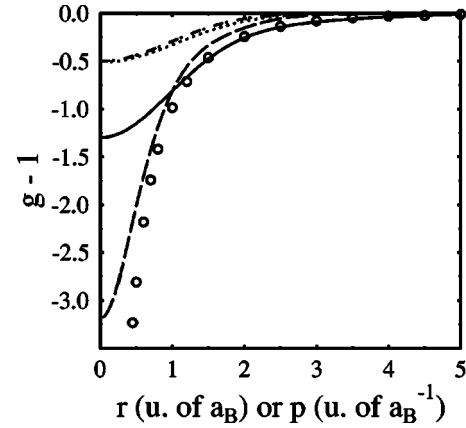


FIG. 5. Correlation functions  $g-1$  for an electron gas in HF and MW approximations: The  $r$  dependence ( $p$  dependence) for HF is shown by the dash-dotted (dotted) line and for MW by the solid (dashed) one. The results in the Debye limit are given by circles. Temperature and density are  $k_B T = 1$  Ry and  $n = 1.35 \times 10^{23} \text{ cm}^{-3}$ .

$$g(r) = g_{\text{id}}(r) + g_{\text{MW}}(r), \quad (39)$$

with  $g_{\text{id}}(r) = 1 + g_{\text{HF}}(r)$  is compared to that in the (classical) Debye limit  $g_D = 1 - e^{-r/\lambda_D} / r$ , which diverges at zero distance. However, here it is not sufficient to take only HF and MW. There follows an unphysical behavior with negative values at small distances. If higher densities and higher temperatures are considered the HF and MW approximations are more justified. In Fig. 7, such a situation is given for an electron gas with temperature  $T = 1 \times 10^6$  K and density  $n = 1.9 \times 10^{24} \text{ cm}^{-3}$ . For comparison, different approximations are shown. In contrast to the Debye approximation, we get positive radial distribution functions at all distances.

## V. CONCLUSION

The aim of this paper was to study the influence of quantum and correlation effects on the different parts of the internal energy as well as on the distribution functions for dense nonideal plasmas using quantum statistical theory. In particu-

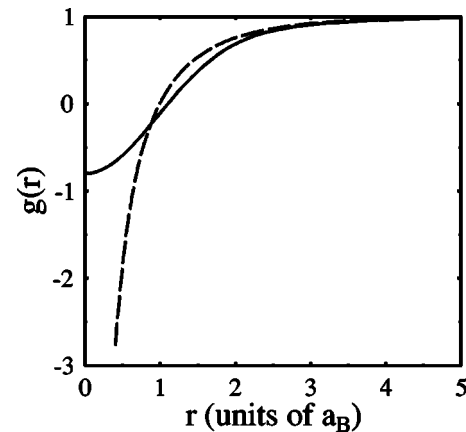


FIG. 6. Radial distribution function  $g(r) = g_{\text{id}}(r) + g_{\text{MW}}(r)$  for an electron gas with  $k_B T = 1$  Ry and  $n = 1.35 \times 10^{23} \text{ cm}^{-3}$  (solid). The corresponding distribution function in the Debye limit is given by the dashed curve.

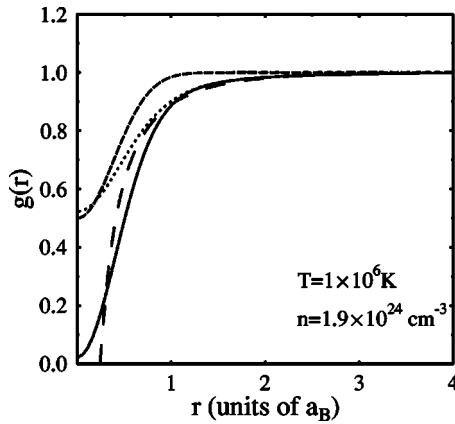


FIG. 7. Radial distribution function  $g(r)$  for an electron gas in different approximations:  $g = g_{id} + g_{MW}$  (solid),  $g_{id}$  (dashed),  $g = 1 + g_{MW}$  (dotted), Debye approximation (long dashed).

lar, the Hartree-Fock and Montroll-Ward approximations were applied to the quantum electron gas. Usually, the correlations in quantum systems lead to an increase of the mean value of the kinetic energy. However, we found that the opposite case is possible, too, i.e., for certain densities and temperatures there is a lowering of the mean kinetic energy as compared to that of an ideal system. This fact has also to be expected for electron-ion plasmas. This special correlation effect follows if the Hartree-Fock term dominates the exchange-correlation contribution to the internal energy. At

the same time the single-particle distribution function is shifted to smaller momenta. The radial distribution is changed as compared to the Debye behavior.

Our calculations confirm results found in path integral Monte Carlo simulations by Pierloni *et al.*, for fully ionized hydrogen, and those recently found by Militzer and Pollock [22] for the electron gas model at finite temperatures. In Ref. [22], hydrogen was considered, too.

In this way, the quantum statistical calculations presented here are of importance for closing the gap between analytical approaches and numerical simulations. Furthermore, the results may be of interest for the understanding of special features, such as cooling of strongly coupled plasmas. Moreover, a detailed investigation of the EOS is of interest for a determination of the speed of sound for the interpretation of solar oscillations, and for the features of the hygoniots from shock experiments [33].

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