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Limiting properties of the radial distribution function in electronic liquids

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Abstract. The static dielectric function of electronic liquids is studied in a wide range of thermodynamic parameters. The local-field correction to the RPA permeability is modelled to satisfy the compressibility sum rule and the short-wavelength exact relation to the zero-separation value of the radial distribution function. The latter is determined by a self-consistency procedure and is shown to verify all known asymptotic conditions.

1. Introduction

A natural approach to the investigation of static correlations in strongly coupled, specifically, inertial fusion plasmas, is based on the separation of electronic and ionic components of the system, so that the interionic interactions are assumed to be screened by the electronic static dielectric function $\varepsilon_e(k)$. In dense systems the latter should be treated beyond the random-phase approximation (RPA), i.e. the calculation of $\varepsilon_e(k)$ involves the electronic static local field correction (LFC) $G_e(k) = G_e(k, \omega = 0)$,

$$\varepsilon_e(k) = 1 + \frac{Q(k, 0)}{1 - G_e(k)Q(k, 0)} \quad (1)$$

where $Q(k, 0)$ is the product $\phi(k)\Pi_e^0(k, \omega)$ at $\omega = 0$, and $\Pi_e^0(k, \omega)$ is the electronic polarization operator in the RPA, $\phi(k) = 4\pi e^2/k^2$.

There exist various approaches to the computation of the LFC $G_e(k)$ (see, e.g. [1]), but mostly they are applicable in specific realms of the system phase diagram. The most notable and far-reaching approach is the modified-convolution approximation (MCA) model suggested by Ichimaru and his co-workers [1]. We present a simple alternative model which is to serve as a basis for future studies of various properties of strongly coupled systems.

The aim of this paper is to propose and check a self-consistent method of calculation of $G_e(k)$ based on its limiting properties and adjusted to the Monte Carlo (MC) data on the one-component plasma (OCP) equation of state (EOS) [2, 3]. Preliminary results obtained within this approach were published elsewhere [4].

2. The model

The interpolating formula for the electronic LFC suggested in [3, 4]

$$G_e(k) = \frac{k^2}{ak_F^2 + bk^2} \quad (2)$$

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incorporates both long- and short-wavelength asymptotic values of $G_e(k)$, $k_F = (3\pi^2 n)^{1/3}$ is the Fermi wavenumber.

In particular,

$$b^{-1} = \lim_{k \rightarrow \infty} G_e(k). \quad (3)$$

The short-range behaviour of $G_e(k)$ in the low-temperature limit has been studied in the papers of Shaw [5] and Kimball [6] (see also [7, 8]). Namely, it has been shown that if $T \rightarrow 0$ in hydrogen-like systems,

$$b^{-1} = 1 - g_e(0) \quad (4)$$

where $g_e(r)$ is the usual electronic radial distribution function. This result is based on the famous ‘cusp’ condition

$$\left(\frac{\partial g}{\partial r} \right)_{r=0} = \frac{1}{a_B} g_e(0) \quad (5)$$

which can be obtained from the s-solution of the two-particle Schrödinger equation at $r = 0$, where a_B is the Bohr radius (see, e.g. [6]).

On the other hand, since $G_e(k \rightarrow \infty)$ involves only the short-range properties of the system, one expects the asymptotic value

$$G_e(\infty) = \lim_{k \rightarrow \infty} G_e(k) \quad (6)$$

to be finite and the relation

$$1 - g_e(0) = \lim_{k \rightarrow \infty} G_e(k) \quad (7)$$

to hold at arbitrary values of temperature T .

The relation (7) stems from the asymptotic value [6]

$$\left(\frac{\partial g(r)}{\partial r} \right)_{r=0} = \frac{3\pi}{8k_F^3} \lim_{k \rightarrow \infty} (k^4 (1 - S_e(k))) \quad (8)$$

where

$$S_e(k) = 1 + \int dr e^{ikr} (g_e(r) - 1) \quad (9)$$

or of electrons.

The long-wavelength behaviour of the latter was studied by Kimball [6, 7] at $T = 0$:

$$1 - S_e(k) = \frac{8k_F^3}{3\pi a_B k^4} (1 - G_e(\infty)) + O\left(\frac{1}{k^6}\right). \quad (10)$$

At $T \neq 0$ the same asymptotic formula (10) also follows from the fluctuation–dissipation theorem,

$$S_e(k) = -\frac{\hbar}{\pi n \phi(k)} \int_0^{+\infty} \coth\left(\frac{\beta \hbar \omega}{2}\right) \text{Im}(\varepsilon_e^{-1}(k, \omega)) d\omega \quad (11)$$

and the static-LFC approximation for the dynamic electronic dielectric function,

$$\varepsilon_e(k, \omega) = 1 + \frac{Q(k, \omega)}{1 - G_e(k)Q(k, \omega)}. \quad (12)$$

In equation (11) \hbar is the Planck constant and β^{-1} is the system temperature T in energy units.

The imaginary part of $\Pi_e^0(k, \omega)$ is exponentially small as $k \rightarrow \infty$ [9], and $\text{Im } \varepsilon_e^{-1}(k, \omega)$ can be substituted by

$$-\frac{\pi}{1 - G_e(\infty)} \delta(1 + (1 - G_e(\infty))\text{Re}Q(k \rightarrow \infty, \omega)) \quad (13)$$

($\delta(z)$ is the Dirac δ -function), while the asymptotic form of $\text{Re}Q(k \rightarrow \infty, \omega)$ is just [9]

$$-(\chi_0^2/3) z^{-2} (u^2 - z^2)^{-1}. \quad (14)$$

Here the Lindhardt notations are introduced:

$$\chi_0^{-2} = \pi k_F a_B \quad z = k/2k_F \quad u = (m\omega)/(\hbar k k_F) \quad (15)$$

where m is the electronic mass.

The expansion (10) has been confirmed by our computations (see further on) with a very high precision.

Returning to the interpolation form (2) for the LFC, one notices that the long-wavelength behaviour of $G_e(k \rightarrow 0) \approx a^{-1}(k/k_F)^2$ is responsible for the screening of a static impurity in the plasma. On the other hand, the parameter a is determined by the system thermodynamic properties via the compressibility sum rule,

$$a^{-1} = \left(\frac{k_F}{k_D}\right)^2 \lim_{k \rightarrow 0} \left(\frac{k_D^2 G_e(k)}{k^2}\right) = \left(\frac{k_F}{k_D}\right)^2 \left(1 - \beta \left(\frac{\partial P}{\partial n}\right)_\beta\right) \quad (16)$$

where $k_D^2 = 4\pi n e^2 \beta$ is the Debye radius and P is the pressure.

The most recent MC data on the OCP EOS [2]

$$P = \frac{n}{\beta} + \frac{\beta U}{3} \equiv \frac{n}{\beta} + \frac{nf(\Gamma)}{3} \quad (17)$$

(U is the system interaction energy and $\Gamma = \beta e^2(4\pi n/3)^{1/3}$) were utilized in this paper with

$$f(\Gamma) = A\Gamma + B + C\Gamma^{-1/3} + D\Gamma^{1/3} \quad (18)$$

and $A = -0.899\,374\,9$, $B = -0.224\,469\,9$, $C = -0.017\,874\,7$, $D = 0.517\,575\,3$.

The interpolation form (17) valid in a very wide region of values of Γ , $0 \leq \Gamma \leq 200$, brought us to a simple algebraic expression for the a parameter,

$$a = -(12\pi^2)^{-1/3} \left(\frac{A}{9} + \frac{B}{12}\Gamma^{-1} + \frac{2C}{27}\Gamma^{-4/3} + \frac{5D}{54}\Gamma^{-2/3}\right)^{-1}. \quad (19)$$

No quantum effects are included in the EOS (17) and, hence, there is discrepancy between (19) (and, thus, equation (2) too) and our desire to apply it to electron liquids under ‘quantum’ thermodynamic conditions.

To diminish the influence of this inconsistency, the parameter $g_e(0)$ (and b of (2)) was determined by a precise self-consistent procedure. In effect, the value of $g_e(0)$ (which itself has a profound physical meaning [1]) was computed via a simultaneous solution of two integral equations,

$$S_e(z) = \sum_{l=-l_1}^{l_1} \frac{\mathcal{P}_e(z, l)}{\varepsilon_e(z, l)} \quad (20)$$

$$g_e(0) = 1 + 12 \int_0^\infty (S_e(z) - 1)z^2 dz. \quad (21)$$

In equation (20) the summation is over the Matsubara frequencies, $v_l = (\pi\Theta l)/(2z)$, and

$$\varepsilon_e(z, l) = 1 + \frac{\Gamma}{(12\pi^2)^{1/3}} \frac{\mathcal{P}_e(z, l)}{z^2} \quad (22)$$

as usually, $\Theta = 2m/(\beta\hbar^2 k_F^2)$, the l_1 -parameter was determined by the numerical precision.

$\mathcal{P}_e(z, l)$ in equation (20) is the dimensionless polarization operator $\Pi_e(k, \omega)$ with the LFC,

$$\mathcal{P}_e(z, l) = \mathcal{P}_e^0(z, l) \left(1 - \frac{\Gamma}{(12\pi^2)^{1/3}} \frac{G_e(z)\mathcal{P}_e^0(z, l)}{z^2} \right)^{-1} \quad (23)$$

$$G_e(z) = \left(b + \frac{a}{(2z)^2} \right)^{-1} \quad b = (1 - g_e(0))^{-1}. \quad (24)$$

The RPA dimensionless polarization operator $\mathcal{P}_e^0(z, l)$ can be calculated (for each value of density and temperature, z and l) by simple integration,

$$\mathcal{P}_e^0(z, l) = \frac{3\Theta}{4z} \int_0^\infty \frac{y dy}{e^{y^2/\Theta-\eta}} \ln \left| \frac{z + y + iv_l}{z - y + iv_l} \right| \quad (25)$$

while the chemical potential η is determined by the normalization condition

$$\int_0^\infty \frac{t^{1/2} dt}{e^{(t-\eta)} + 1} = \frac{2}{3} \Theta^{-3/2}. \quad (26)$$

We studied the asymptotic behaviour of the model parameter $g_e(0)$ and compared (where possible) our results with those of [1], etc.

The self-consistency procedure, equations (20), (21), proved to be numerically stable, and the resulting values of $g_e(0)$ were independent of the initiation points. The latter did influence the number of iterations slightly, which varied (for the data given below) between 2 and 5 to ensure the absolute error in the determination of $g_e(0)$ was between 10^{-2} and 10^{-3} .

3. Results and conclusions

The results of the above self-consistent procedure to evaluate the zero-separation value of the electronic radial distribution function $g_e(0)$ are provided in figure 1. Some additional points are also given in table 1, where, in particular, we present the values of $g_e(0)$ for

Table 1. The zero-separation value of the electronic pair correlation function $g_e(0)$ for various values of electronic density and temperature. The values of $g_e^Y(0)$ (last column) are calculated according to (27) [11]. The values of the parameters Γ , Θ and r_s are given for reference.

n_e (10^{24} cm $^{-3}$)	T (10^5 K)	Γ	Θ	r_s	$g_e(0)$	$g_e^Y(0)$
0.2579	1.715	1.0	1.0	1.84	0.026	0.1635
1.6100	6.315	0.5	1.08	1.00	0.1262	0.2661
2.063	3.429	1.0	0.5	0.92	0.1633	0.2792
1.611	1.579	2.0	0.27	1.00	0.1903	0.2662
2.517×10^1	1.579×10^1	0.5	0.4342	0.40	0.3198	0.3856
2.579×10^2	1.715×10^1	1.0	0.1	0.18	0.4376	0.4430
2.579×10^5	1.715×10^3	0.1	0.1	0.02	0.4919	0.4939
2.160×10^3	3×10^3	0.01	4.24	0.09	0.6960	0.4709
1.250	2.5×10^2	0.01	50.00	1.09	0.9850	0.2525

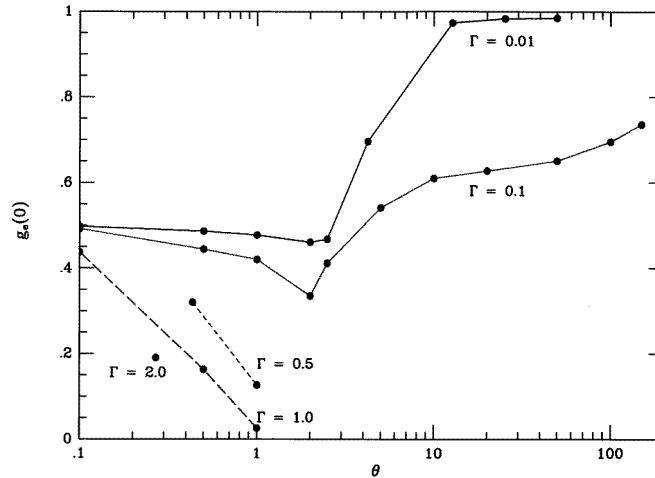


Figure 1. The zero-separation value of the pair correlation function $g_e(r)$ in the electron liquid as a function of the degeneracy parameter Θ and for $\Gamma = 2.0$ (one point), $\Gamma = 1.0$ (long broken), $\Gamma = 0.5$ (short broken), $\Gamma = 0.1$ (dotted) and $\Gamma = 0.01$ (full). Points represent the results of the present model, the lines are drawn to distinguish different values of the coupling parameter Γ .

the electronic density $n_e = 1.60 \times 10^{24} \text{ cm}^{-3}$ and temperature $T = 1.579 \times 10^5 \text{ K}$ and $T = 6.315 \times 10^5 \text{ K}$, i.e. $r_s = 1.0$ and $\Theta = 0.27$ and $\Theta = 1.0$, respectively, r_s being, as usually, the Wigner–Seitz radius in the units of a_B , $r_s = \Gamma\Theta/0.543$. These values are the only ones for which we could carry out the comparison with the results published by Tanaka *et al* [10]. The values of $g_e(0)$ (0.1903 and 0.1262) coincide with the data of [10] corresponding to the approximation, when the electron–ion LFC was set to be zero. This coincidence is not astonishing, since here we virtually consider the one-component electronic system.

The self-consistency procedure also permitted us to calculate the static structure factor of electrons, these results are provided in figure 2 for three characteristic pairs of values of the parameters Γ , Θ and $g_e(0)$ (see table 1).

For the sake of comparison we also present in table 1 the corresponding values of $g_e(0)$ calculated according to the formula, obtained by Yasuhara [11] through a resummation of the electron–electron ladder diagrams,

$$g_e(0) = [q/I_1(q)]^2/8 \quad (27)$$

where $q \simeq 1.629\sqrt{r_s}$ and $I_1(q)$ is the first-order modified Bessel function.

Notice, that though we do not include spin effects (bearing in mind that they would manifest themselves only in magnetized Coulomb systems) it is obvious that $g_e(r=0) \neq 0$ only for two electrons with opposite spins. Thus, within the Hartree–Fock approximation when the exchange effects prevail over those of the Coulomb interaction, the value of $g_e(0)$ is just $\frac{1}{2}$. This high-degeneracy limiting value is actually the asymptotic value of $g_e(0)$ resulting from our calculations as $\Theta \rightarrow 0$, and the smaller Γ , the quicker $g_e(0)$ approaches the quantum ideal-gas value $g_e^{HF}(0) = \frac{1}{2}$.

On the other hand, as Θ grows, the system becomes more and more classical from the statistical point of view, when no spin effects could manifest themselves. And if, in addition, the Coulomb interaction is relatively small ($\Gamma \simeq 0.01$), the value of $g_e(0)$ approaches the

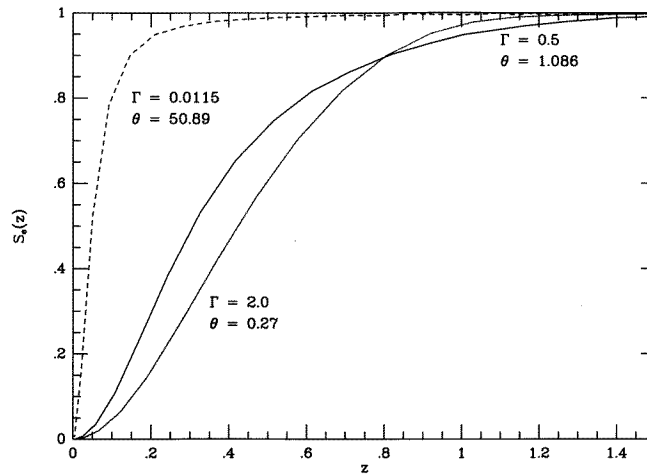


Figure 2. The self-consistent electronic static structure factor $S_e(z)$ ($z = k/(2k_F)$) for three characteristic pairs of values of density and temperature: $\Gamma = 0.01$, $\Theta = 50.0$ (broken curve); $\Gamma = 0.5$, $\Theta = 1.0$ (full curve); $\Gamma = 2.0$, $\Theta = 0.27$ (dotted curve). For other parameters, see table 1.

classical ideal-gas limiting value of 1 already at $\Theta \simeq 10$. In systems with stronger Coulomb interactions ($\Gamma \simeq 0.1$) this asymptotic value is reached at higher values of $\Theta > 150$.

In weakly coupled electron liquids with $\Gamma \gtrsim 0.5$ the exchange effects resulting in attraction of electrons with antiparallel spins are compensated for by the Coulomb repulsion, and in such systems the value of $g_e(0)$ decreases significantly with growing Γ . Strong Coulomb coupling ($\Gamma \gtrsim 1$) can (asymptotically) reduce the value of $g_e(0)$ to zero (pure Coulomb repulsion). In our model it appears that the exchange contribution to $g_e(0)$ is underestimated, so that this reduction already occurs at about $r_s \simeq 1.84$, which is 22% higher than the value stemming from the high-density expansion of the Yasuhara's formula [11], $q = 2$.

In conclusion, the dielectric formalism is applied to the description of electron one-component liquids and a simple model expression for the electronic local-field correction satisfying the compressibility sum rule and the exact short-wavelength limiting ('cusp') condition is studied. The long-wavelength behaviour of the LFC is adjusted to the MC-fitted equation of state. The model parameter $g_e(0)$ (the zero-separation value of the electronic radial distribution function) is obtained by the self-consistency procedure in a wide range of thermodynamic parameters and is shown to possess physically reasonable limiting properties.

Nevertheless, further studies of $g_e(0)$ might be carried out to include low-temperature [12] and dynamic effects.

In addition, to improve the physical self-consistency of our approach, one needs the quantal EOS, either theoretical or numerical (obtained, e.g. within a quantum-statistical variant of the MC method).

The static LFC determined here is expected to become a reliable tool in the determination of static and thermodynamic characteristics of dense Coulomb systems at intermediate and high values of temperature. Their dynamic and kinetic properties can be studied within an alternative approach to those pointed out by Sturm in his recent paper [13], and based on the construction of the plasma dynamic dielectric function by the method of frequency moments using all known exact relations and sum rules (see [4, 14] and references therein).

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