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2009 J. Phys. A: Math. Theor. 42 214053

(http://iopscience.iop.org/1751-8121/42/21/214053)

J. Phys. A: Math. Theor. **42** (2009) 214053 (4pp) doi:10.1088/1751-8113/42/21/214053

Ion structure in dense plasmas: MSA versus HNC

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Received 23 September 2008, in final form 27 October 2008
Published 8 May 2009
Online at stacks.iop.org/JPhysA/42/214053

Abstract
We present results for the ionic structure in dense, moderately to strongly coupled plasmas using two models: the mean spherical approximation (MSA) and the hypernetted chain (HNC) approach. While the first method allows for an analytical solution, the latter has to be solved iteratively. Independent of the coupling strength, the results show only small differences when the ions are considered to form an unscreened one-component plasma (OCP) system. If the electrons are treated as a polarizable background, the different ways to incorporate the screening yield, however, large discrepancies between the models, particularly for more strongly coupled plasmas.

PACS numbers: 61.20.Gy, 52.27.Gr, 52.59.Hq

1. Introduction

Structural properties of dense plasmas are of great importance for the understanding of astrophysical objects as giant gas planets [1] and to achieve the aim of inertial confinement fusion [2] since the well-pronounced short-range structure created by the strong Coulomb interactions influences the equation of state and transport properties. Moreover, the ionic structure plays an essential role when determining the plasma properties by means of x-ray scattering as a diagnostic tool [3–5].

The strength of the interaction between the ions is given by the classical coupling parameter $\Gamma_{ii} = Z^2e^2/k_BTa_i$ where $a_i = (3/4\pi n_i)^{1/3}$ is the mean distance between ions with density n_i. The electrons in dense plasmas are often partially to highly degenerate, i.e., $n_e\Lambda_e^3 = n_e(2\pi\hbar^2/m_ek_BT)^{3/2} \geqslant 1$. Due to the smaller charge and/or high degeneracy, the electron–ion interaction is mostly weak. Thus, it can be treated within linear response which yields linearly screened ion–ion interactions [6].

The spatial microscopic arrangement of the ions in the plasma can be described by the pair distribution function $g_{ii}(r)$ or the static structure factor $S_{ii}(k)$. These quantities are connected

by Fourier transformation

$$S_{ab}(\mathbf{k}) = \delta_{ab} + \sqrt{n_a n_b} \int \mathrm{d}\mathbf{r}[g_{ab}(r) - 1] \exp(\mathrm{i}\mathbf{k} \cdot \mathbf{r}). \tag{1}$$

Here, two approaches for the ionic structure in dense plasmas are discussed. Both are based on the Ornstein Zernike relation [7], but use a different closure relation. Although the mean spherical approximation (MSA) introduces more drastic approximations, it has the advantage of an analytical solution while the hypernetted chain (HNC) approach relies on an iterative numerical treatment. The comparison shows when MSA can be used and when the HNC method must be applied. We will consider the plasma electrons in two models: (i) uniform and structureless (one component plasma (OCP) model) and (ii) as a polarizable background (Yukawa model).

2. Theoretical models for the ionic structure

The classical integral equation approach is based on the Ornstein Zernike relation [7]

$$h_{ab}(\mathbf{r}) = c_{ab}(\mathbf{r}) + \sum_c n_c \int \mathrm{d}\bar{\mathbf{r}}\, c_{ac}(\bar{\mathbf{r}}) h_{cb}(|\mathbf{r} - \bar{\mathbf{r}}|), \tag{2}$$

which connects the direct and total correlation functions, $c(r)$ and $h(r) = g(r) - 1$, respectively. The needed closure relation is obtained by cluster expansion to be [6]

$$g_{ab}(r) = \exp\{-\beta V_{ab}(r) + h_{ab}(r) - c_{ab}(r) + B_{ab}(r)\}. \tag{3}$$

These two equations fully determine the structure in classical systems. Unfortunately, the bridge functions $B(r)$ are unknown and must be approximated.

2.1. The hypernetted chain (HNC) approach

If the bridge functions $B(r)$ are set to zero in equation (3), the HNC closure relation follows. The system of equations (2) and (3) is now fully defined and can be solved iteratively, even for many ion species [8]. The solutions are in good agreement with molecular dynamics (MD) and Monte Carlo (MC) simulations for Coulomb-like potentials and coupling strengths up to $\Gamma_{ii} \leqslant 100$ [9].

OCP calculations use bare Coulomb interactions $V_{ii}^C(r) = Z^2 e^2 / r$. For most systems, screened ion–ion interactions are more realistic. Here, we consider only linear screening, i.e., weak electron–ion interactions, that yields the well-known statically screened Coulomb or Debye potential [13]:

$$V_{ii}^D(r) = \frac{Z^2 e^2}{r} \exp(-\kappa_e r) \qquad \text{with} \qquad \kappa_e^2 = \frac{4e^2 m_e}{\pi \hbar^3} \int_0^\infty \mathrm{d}p\, f_e(p). \tag{4}$$

The inverse screening length κ_e is here defined by the Fermi distribution of the electrons $f_e(p)$ to allow for degeneracy. This definition includes the classical limit (inverse Debye length) as well as Thomas–Fermi screening for low temperatures. Since we are interested in equilibrium properties, the electron and ion temperatures used are the same.

2.2. Mean spherical approximation (MSA)

Another closure relation for the Ornstein Zernike equation is given by the mean spherical approximation (MSA) designed for systems with hard core repulsions,

$$g_{ii}(r) = 0 \qquad \text{for} \quad r < \sigma_c \qquad \text{and} \qquad c_{ii}(r) = -\beta V_{ii}^C(r) \qquad \text{for} \quad r > \sigma_c. \tag{5}$$

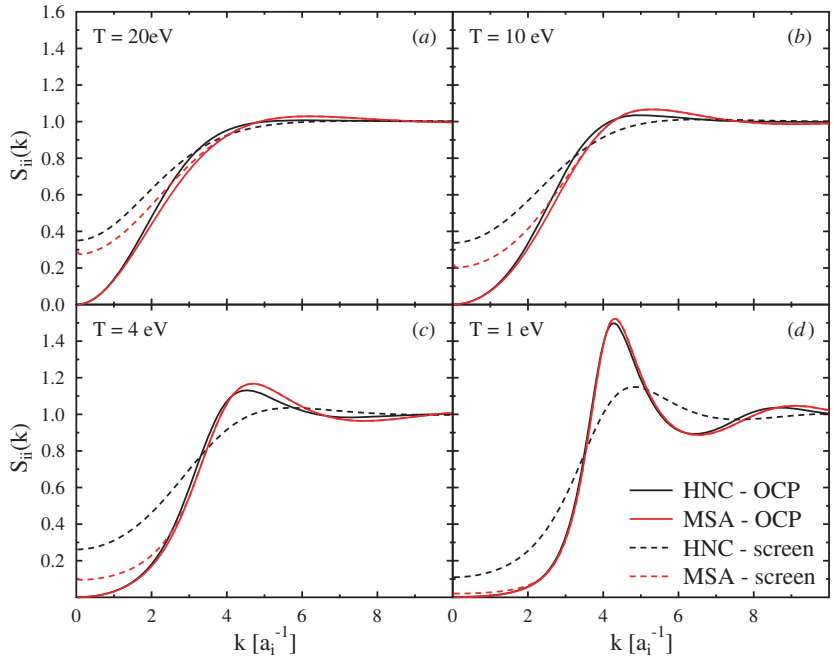

Figure 1. Static ion–ion structure factore $S_{ii}(k)$ for doubly charged ions with a density of $n_i = 1.5 \times 10^{23}$ cm^{-3} at different temperatures. The electron screening length is calculated self-consistently for the temperatures given from equation (4).

(This figure is in colour only in the electronic version)

Thus, this model considers the plasma ions as positively charged hard spheres with a diameter σ_c that interact via Coulomb forces in a uniform neutralizing background of the electrons. For such a OCP-like model system, one can find an analytical solution [10, 11]. The ion–ion structure factor is then given by $S_{ii}^{\mathrm{OCP}}(k) = [1 - c_{ii}(k; \sigma_c)]^{-1}$, where the direct correlation function is a functional of the cut-off parameter σ_c. In the MSA, this quantity is determined by requiring a continuous pair distribution function at the hard-sphere boundary [12].

The upper solution must be modified if screening by the electrons should be considered. To keep the possibility of an analytical solution, one applies a weak empty-core pseudo-potential of the form $V_{ei}(k) = -(Ze^2/k^2)\cos(k\sigma_c/2)$ for the electron–ion interactions. This potential yields the screening function [14–16]

$$f(k) = \frac{\kappa_i^2}{k^2}\cos^2(k\sigma_c/2)\left[\frac{1}{\varepsilon(k)} - 1\right] = -\frac{\kappa_i^2}{k^2}\cos^2(k\sigma_c/2)\left[\frac{\kappa_e}{k^2 + \kappa_e^2}\right], \tag{6}$$

where $\kappa_i = (4\pi Z n_e e^2/k_B T)^{1/2}$ is the inverse of the classical ion Debye length and $\varepsilon(k)$ the dielectric function of electrons. The latter has been used in the long wave length limit of the random phase approximation to obtain the second form.

The ion–ion structure factor for the screened ionic subsystem is then given by

$$S_{ii}(k) = \frac{S_{ii}^{\mathrm{OCP}}(k)}{1 + f(k)S_{ii}^{\mathrm{OCP}}(k)}. \tag{7}$$

To avoid an unphysical behaviour of $S_{ii}(k)$ and to ensure smooth electron wavefunctions, the electron–ion pseudo-potential $V_{ei}(k)$ is truncated after the first node [16].

3. Comparison of the results from the HNC and MSA approaches

Static ionic structure factors calculated from the theories presented above are plotted in figure 1 for plasmas with approximately solid density, an ion charge of $Z = 2$ and different temperatures. The results are compared for OCP and screened systems.

In the OCP model, the structure factors from HNC and MSA calculations are in good agreement which holds for all coupling strength Γ_{ii}. The more approximate MSA gives slightly higher and shifted peaks. This documents that the extra cut-off in the MSA has only a minor effect on the ionic structure. Since direct classical simulations, such as MD and MC, showed good agreement with HNC results [8, 9], the MSA can be considered to be reasonably accurate for OCPs up to high coupling strengths.

The screening of the Coulomb interactions yields to the expected characteristics: the structure factors increase for small wave vectors k and the oscillations are damped due to the weaker interactions at larger separations. In general, the structure is more affected by screening when calculated by the HNC equations than within the MSA approach. These differences strongly increase with coupling strength where the inverse screening length κ_e becomes larger as well. For the moderately coupled ions in figures 1(*a*) and (*b*) both approaches give similar results. On the other hand, the results shown in figures 1(*c*) and (*d*) display qualitative differences between the two approaches. This behaviour is connected to the way how screening is treated within the MSA. Here, the highest wave number, where the structure factor is screened (first node in the electron–ion pseudo-potential) becomes smaller with coupling strength. In figures 1(*c*) and (*d*), this cut-off is already less than the first peak of the structure factor $S_{ii}(k)$. Accordingly, the screened MSA coincides with the OCP result for most k values and spatial correlations are overestimated.

Our results show that, for plasmas with strongly coupled and screened ions, the MSA may fail to incorporate the crucial effect of screening in the whole wave number space due to the truncation of the screening function at very small k. An interpretation of the ion feature in the x-ray scattering signal [4] with the MSA should thus be limited to moderately coupled or weakly screened plasmas similar to those in [3, 5].

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