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Ion microfield distributions for strongly coupled Yukawa fluid combining VMHNC and APEX methods

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Abstract

The low-frequency component of electric microfield distribution is calculated for a wide range of ion-ion coupling and electron screening parameters in the Yukawa fluid domain. We use a modified APEX method incorporating the VMHNC approach. The results are represented by analytic fitting formulas suitable for applications. The influence of the ion microfield distributions on the Rosseland mean opacity of iron and spectral line shape calculations is presented and discussed.

Introduction

In dense plasmas, the electric field created by the perturbators (electrons and ions) at the position of the radiator (atom or ion) affects significantly the spectral line shape by modifying his atomic structure. For many applications, the perturbing ions are stationnary over the corresponding radiating times [1]. Consequently, the problem can be reduced to the determination of the probability distribution of the low-frequency component of perturbing electric fields [2].

Since the pioneering work of Holtsmark [3], several methods have been developed to describe the ion microfield distributions but they are often limited to weakly or moderatly coupled plasmas. A computationnaly efficient method, valid for weakly and strongly coupled regimes, is the adjustable-parameter exponential (APEX) treatment ([4] and references therein). It involves a noninteracting quasiparticule picture of the screened ions, in which the hypernetted chain (HNC) integral equations are used to calculate the radial pair distribution function [5].

In this paper, we extend the APEX approximation incorporating the variational modified HNC approach (VMHNC) [6, 7], in the aim to generate the ion microfield distributions more accuratly over the fluid domain for a wide range of the dimensionless coupling and screening Yukawa parameters (Γ, κ). Then, we propose analytic fitting formulas with respect to Γ and κ that reproduce the APEX-VMHNC calculations, suitable for applications. Finally, we discuss the influence of the microfields on the Rosseland mean opacity of iron and spectral line shape calculations.

The APEX-VMHNC method

We quote here the main ingredients used in the APEX-VMHNC formalism. We consider a one-component plasma (OCP) constitued of N identical ions immersed in a uniform neutralizing background (electrons), in thermodymanic equilibrium at a temperature T, where the interparticle interactions are modeled with the following Yukawa (Y) potential:

$$V(r) = \frac{(Z^*e)^2}{r} e^{-r/\lambda_D} \tag{1}$$

Z^* and e are the residual ion charge and the electron charge. $\lambda_D = (k_B T/4\pi\rho_e e^2)^{1/2}$ is the Debye wavelength, with k_B the Boltzmann constant and ρ_e the electron density ($\rho_e = Z^*\rho_i$). The YOCP model can be characterized by the couple of dimensionless ion-ion coupling and electron screening parameters which are $\Gamma = (Z^*e)^2/k_B T r_{ws}$ and $\kappa = r_{ws}/\lambda_D$. $r_{ws} = (3/4\pi\rho_i)^{1/3}$ is the Wigner-Seitz radius, where ρ_i is the ion density. The APEX approximation is based on a noninteracting quasiparticule representation of the screened ions, introducing effective single particle electric fields with an adjustable parameter α:

$$E_{APEX}(r) = Z^*e\frac{(1+\alpha r)}{r^2} e^{-\alpha r} \tag{2}$$

With the knowledge of the radial pair distribution function $g(r)$, the parameter α is then adjusted to satisfy the local-field constraint and the second moment rule of the microfield distribution [8]. That way, this approach provides a scheme for evaluating the ion microfield distributions. Here, we use the VMHNC approach to calculate $g(r)$. Thus, we take into account the Bridge function properties in the standard integral equations of simple fluid theory:

$$g(r) = \exp\big(-V(r)/k_B T + h(r) - c(r) + B(r)\big) \tag{3}$$

$h(r) = g(r) - 1$ is the total correlation function and $c(r)$ the direct correlation function defined by the Ornstein-Zernike equation. The method of solution is to set $B(r) = B_{HSPY}(r,\eta)$, where $B_{HSPY}(r,\eta)$ is the Percus-Yevick hard-sphere (HS) Bridge function. Then, the best free energy of the system is determined by minimization with respect to $g(r)$ and the packing fraction η of the auxiliary HS system. Finally, we improve the APEX-VMHNC calculations incorporating the nearest neighbor model [9] to describe the large fields of the distribution, and the Levin-type transformation [10] to accelerate the convergence of the integration of oscillatory functions.

Applications

In the aim to having ion microfield calculations easily available in numerical codes for applications, we have established an analytic expression that reproduces the APEX-VMHNC results:

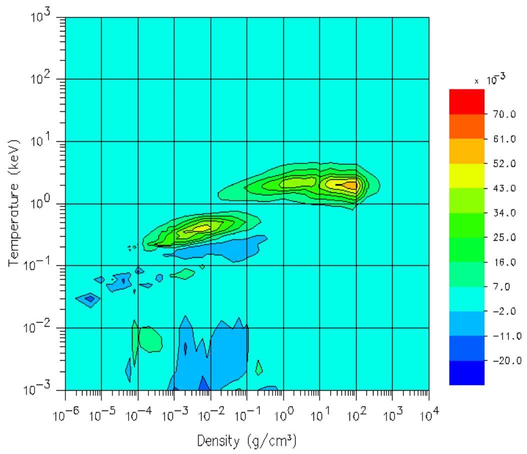

Figure 1: Relative variation between iron Rosseland mean opacity calculations including the ion microfield distributions (4) and calculations without microfields.

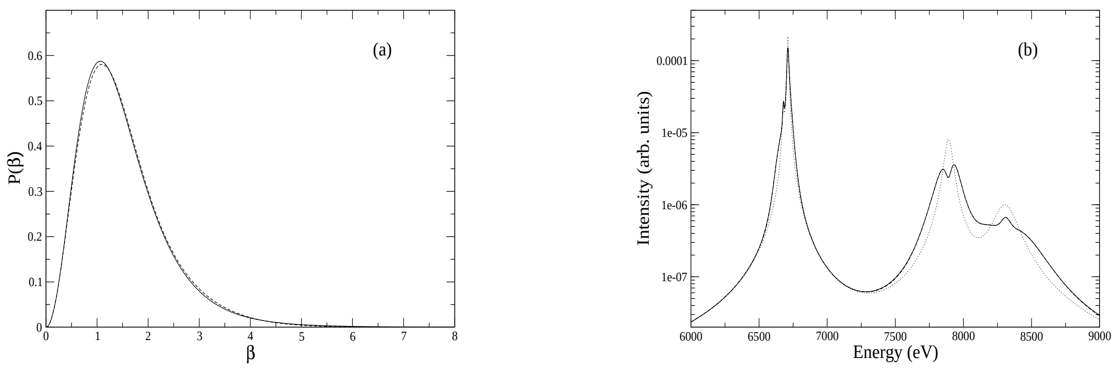

Figure 2: (a) Microfield distribution function obtained by the APEX-VMHNC method (full line) and by the analytic fitting formula (4) (dashed line). (b) Fe He-α,β,γ line shapes including the various microfield distributions. The spectral line including only electronic contribution is also plotted (dotted line). Plasma conditions: $T = 2$ keV, $\rho = 100$ g/cm^3 ($\Gamma = 6.2$, $\kappa = 0.9$).

$$P(\beta) = \beta^2 \left(A_0 e^{-A_2 \beta^{A_4}} + A_1 e^{-A_3 \beta^{A_5}}\right)/C_N \tag{4}$$

C_N is the normalization constant. $\beta = E/E_0$ is the dimensionless electric field with $E_0 = Z^{*2/3} e/r_{ws}^2$. The coefficients $A_{n=0\to5}$ are tabuled polynomial or rational functions with respect to the two adapted parameters $t^* = \Gamma/\Gamma_M$ and $k^* = 1/(\kappa+1)$. Γ_M is the ion-ion coupling at the solid-liquid melting boundary [11]. That way, the analytic approximation (4) is valid over a wide range of the Yukawa fluid domain, i.e. at $\Gamma \le \Gamma_M$ and $\kappa \le 5$.

We have integrated our analytic fitting formula (4) in a spectral opacity code. We plot in Fig. 1 the relative variation obtained between iron Rosseland mean opacity calculations including ion microfields and calculations without microfields. We observe an influence of few percents of the microfields on the mean opacity values. A maximum of 6% is quoted at $T = 2$ keV and $\rho = 100$ g/cm^3. At these plasma conditions, we plot in Figs. 2(a) and 2(b) the corresponding ion microfield distribution function and spectral line shapes, respectively. The line shape calculations have been made using the frequency fluctuation model [12], where the electron broadening is modeled by the modified semi-empirical model [13]. Agreement between the APEX-VMHNC calculations and analytic results is excellent. We observe a significant modification of the line shapes when we include the ionic contribution.

Conclusion

The APEX-VMHNC method provides an efficient way to compute ion microfield distribution functions on a wide range of the Yukawa fluid domain. The analytic fitting formula proposed to reproduce the APEX-VMHNC calculations is accurate, suitable for applications, and valid for $\Gamma \leq \Gamma_M$ and $\kappa \leq 5$. The Stark effect created by the ion microfields modifies only some percents the Rosseland mean opacity calculations of iron, but it responsible for a non negligeable broadening and splitting of the non perturbated line shapes.

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