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# Dynamic properties of MD model plasmas

I.M. Tkachenko*,** and J. Alcober*

* *Department of Applied Mathematics, Polytechnic University, 46022 Valencia, Spain*
** *Mediterranean University Center of Science and Technology, 46022 Valencia, Spain*

**Abstract.** The classical method of moments is applied to study the dynamic characteristics of model hydrogen plasmas. The employment of the effective potential improves the overall agreement with the MD data.

## 1. INTRODUCTION

Simulation of electron-ion plasmas by the classical molecular dynamics (MD) method requires the employment of effective potentials preventing the Coulomb collapse. Well-known extensive studies of dynamic properties of strongly coupled hydrogen plasmas by Hansen et al. [1] were carried out using the pairwise potential of C. Deutsch et al. [2] $\Phi_{eff}$. Since then a number of theoretical studies (see: [3], [4], [5], to mention a few) were undertaken to compare their results with those of the molecular simulation. All of them did not take into consideration the effective potential $\Phi_{eff}$.

The aim of the present work is to determine the influence of $\Phi_{eff}$ vs. the pure Coulomb potential, on the plasma properties.

## 2. THE STRUCTURE FACTOR

The plasma dynamic structure factor *"charge-charge" $S(k,\omega)$* is related to the system dielectric function $\varepsilon(k,\omega)$ via the fluctuation-dissipation theorem. The loss function $L(k,\omega;h) \equiv -\operatorname{Im}\varepsilon^{-1}(k,\omega)$ is reconstructed [5] within the classical method of moments [6] on the basis of sum rules and exact relations:

$$L(k,\omega;h) = \frac{\omega_p^2 \omega h\left(\omega_2^2 - \omega_1^2\right)}{\omega^2\left(\omega^2 - \omega_2^2\right)^2 + h^2\left(\omega^2 - \omega_1^2\right)^2}, \tag{1}$$

so that

$$\frac{S(k,\omega)}{S(k,0)} = \frac{\{\beta\hbar\omega/[1-\exp(-\beta\hbar\omega)]\}h^2\omega_1^4}{\omega^2\left(\omega^2 - \omega_2^2\right)^2 + h^2\left(\omega^2 - \omega_1^2\right)^2} \quad , \tag{2}$$

where $\beta^{-1}$ is the plasma temperature, $h$ is the positive "decay" parameter, and $\omega_i^2$ ($i$ = 1, 2) are successive ratios of the loss function frequency moments [7]:

$$C_\nu(k) = -\pi^{-1}\int_{-\infty}^{\infty}\omega^{\nu-1}\operatorname{Im}\varepsilon^{-1}(k,\omega)d\omega \quad \nu = 0,1,2,\ldots;$$
$$\omega_1^2 = C_2/C_0 = \omega_p^2\left[1-\varepsilon^{-1}(k,0)\right]^{-1},$$
$$\omega_2^2 = C_4/C_2 = \omega_p^2\left[1+Q(k)\right] \quad .$$

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Here $\omega_p$ is the plasma frequency,

$$Q(z)=3(k/k_D)^2+\sqrt{\pi/18}\left(\lambda_T^3k^2/\lambda_L\right)+\left(\lambda_T^2k^4/k_D^2\right)+$$
$$+\frac{1}{3\pi^2 n}\int_0^\infty p^2 S_{ei}(p)dp+\frac{1}{6\pi^2 n}\int_0^\infty p^2\left[S_{ee}(p)-1\right]f(p,k)dp,$$

$$f(p,k)=\frac{5}{8}-\frac{3p^2}{8k^2}+\frac{3\left(k^2-p^2\right)^2}{16pk^3}\ln\left|\frac{p+k}{p-k}\right|,$$

$$k_D^2=4\pi ne^2\beta,\quad \lambda_T=\sqrt{\hbar^2\beta/2m_e},\quad \lambda_L=2e^2\beta/3,$$

$m_e$ and $e$ are electronic mass and charge, $n = n_e = n_i$ is the particles (electrons or ions) number density. The species static structure factors $S_{ab}(k)$ ($a$, $b$ = $e$, $i$) and the static dielectric function $\varepsilon(k,0)$ were calculated self-consistently beyond the random-phase approximation using the local-field correction satisfying the Kimball condition and the compressibility sum rule [5], [8], [9], [10]. In particular, the ionic characteristics were estimated by the algorithm of [11] on the basis of our "electronic" results [10]:

$$G_i(k)=G_i(k)/\varepsilon_e(k,0),$$
$$S_{ii}(k)=\left\{1+\left(k_D^2/k^2\right)\left[\varepsilon_e^{-1}(k,0)-G_i(k)\right]\right\}^{-1},$$
$$S_{ei}(k)=\left[1-\varepsilon_e^{-1}(k,0)\right]S_{ii}(k),$$
$$S_{ee}(k)=S_e(k)+\left[1-\varepsilon_e^{-1}(k,0)\right]S_{ei}(k);$$

and

$$\varepsilon(k,0)=1+\sum_{a=e,i}\frac{\Phi_{aa}(k)\Pi_a^0(k,0)}{1-\Phi_{aa}(k)G_a(k)\Pi_a^0(k,0)},$$
$$\Phi_{aa}(k)=4\pi e^2\phi_{aa}^2(k)/k^2,$$

$\Pi_{aa}^0(k,0)$ being the RPA static polarization functions [10]. The form-factors corresponding to the effective potential $\Phi_{eff}$ of [2] are determinated by the interacting particles charge numbers and their masses $m_a$:

$$\phi_{aa}(k)=\left[1+\beta\hbar^2k^2/\pi m_a\right]^{-1/2}. \tag{3}$$

Notice that the ions were considered classically within the classical statistics.

## 3. RESULTS

We employed the procedure of maximization of the Shannon entropy

$$S(k;h)=-\int_0^\infty L(k,\omega;h)\ln L(k,\omega;h)d\omega$$

to find the decay parameter $h$. The results of our calculations for the Langmuir mode dispersion (Table 1) and the dynamic structure factor *"charge-charge"* (Fig. 1) reproduce the MD data quite well. We observe that if the potential $\Phi_{eff}$ is used to compute the plasma characteristics beyond the random-phase approximation , the agreement improves consistently. Otherwise, if the decay parameter $h$ is adjusted to reproduce one "experimental" (MD) point, the level of agreement is similar, or even better, e.g. in the case d) of Fig. 1, but the results are no longer coherent with respect to the effective potential $\Phi_{eff}$ introduction (thus we do not present the results of this adjustment here). We conclude that our results confirm the effectiveness of $\Phi_{eff}$ for the simulation of Coulomb systems, and seem to imply the consistency of the conjecture of Ref. [12] on the possibility to obtain the value of the method-of – moments decay parameter by the Shannon entropy maximization.

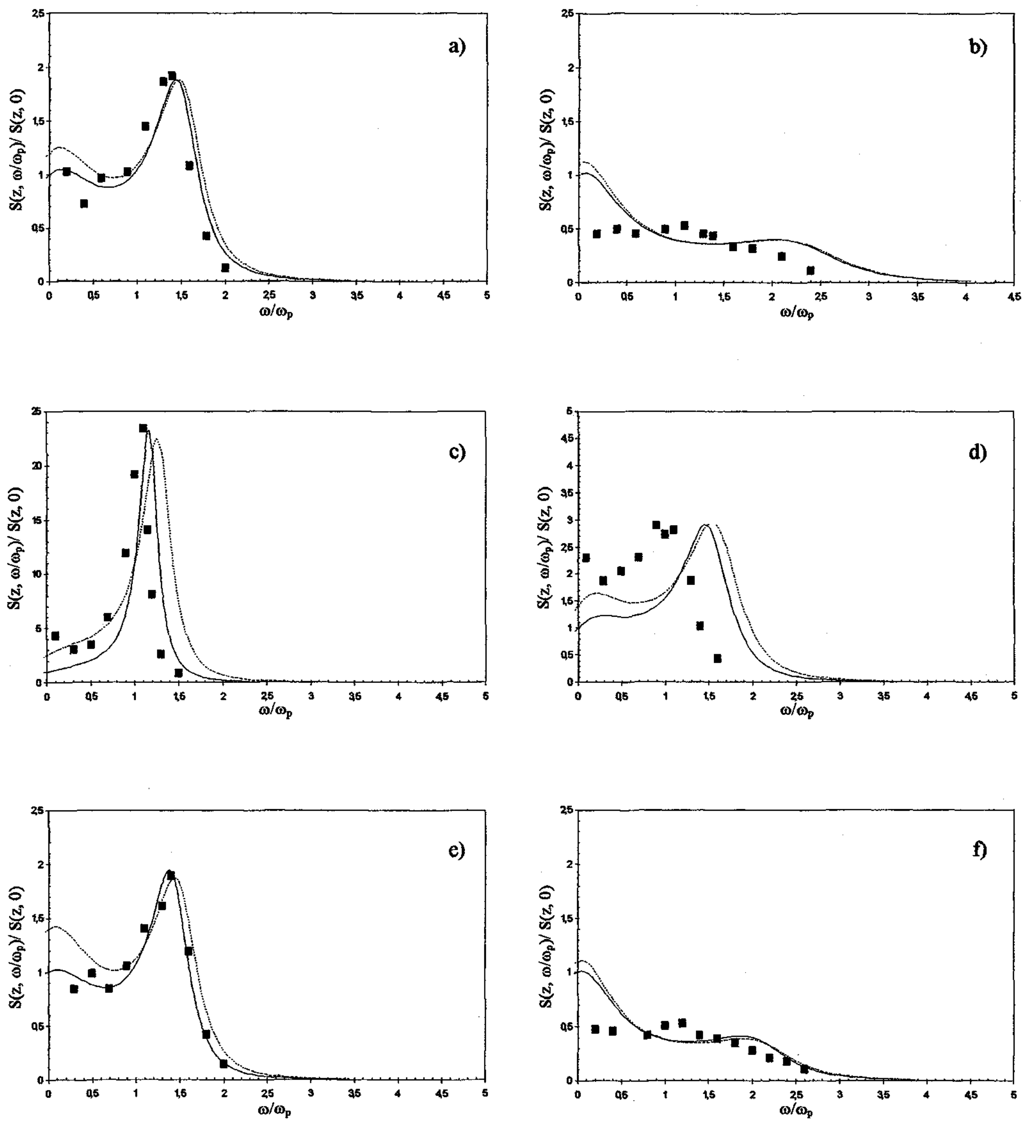


**Fig. 1.** Results obtained using the Shannon entropy maximization to find the appropriate $h$ parameter. Dots are MD results, solid lines are with and dashed lines are without the effective interaction form-factors included. a) $\Gamma$=0.5, $\Theta$=0.434292, $q$=0.78; b) $\Gamma$=0.5, $\Theta$=0.434292, $q$=1.35; c) $\Gamma$=2, $\Theta$=0.2714, $q$=0.78; d) $\Gamma$=2, $\Theta$=0.2714, $q$=1.35; e) $\Gamma$=0.5, $\Theta$=1.0855, $q$=0.78; e) $\Gamma$=0.5, $\Theta$=1.0855, $q$=1.35; with $q=k(4\pi n_e/3)^{-1/3}$.

**Table 1.** Corresponding MD and theoretical (with and without the effective form-factors included) values of the Langmuir frequency $\omega_L(k)$.

| Fig. | $\omega_L/\omega_p$ MD | $\omega_L/\omega_p$ | |
|---|---|---|---|
| | | $\phi_{aa}(k)=1$ | $\phi_{aa}(k)$ of Eq. (3) |
| 1.a) | 1.4 | 1.44182 | 1.47406 |
| 1.c) | 1.1 | 1.1554 | 1. 25156 |
| 1.d) | 1.1 | 1.46235 | 1.54128 |
| 1.e) | 1.4 | 1.37877 | 1.43855 |

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