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Monte Carlo Simulations of the Yukawa One-Component Plasma

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The excess free energy f of the Yukawa one-component plasma is investigated by means of Monte Carlo simulations. These simulations are performed in the canonical ensemble within hyperspherical boundary conditions and f is computed for various values of the coupling parameter Γ in the range $0.1 \leqslant \Gamma \leqslant 100$ and of the screening parameter α^* in the range $0.1 \leqslant \alpha^* \leqslant 6$.

KEY WORDS: Yukawa potential; strongly coupled plasmas; Monte Carlo simulations.

I. INTRODUCTION

Recently, many models involving Yukawa interactions have been proposed to study the thermodynamic and structural properties of various systems such that dusty plasmas,[1–4] dense plasmas,[5, 6] and colloids.[7, 8] In the present paper, we consider the case of the Yukawa one-component plasma (YOCP), i.e., a system made of N identical point charges q interacting via an effective Yukawa pair-potential $v_\alpha(r) = \exp(-\alpha r)/r$, where α is the so-called screening parameter. The hamiltonian of an YOCP enclosed in a volume Λ of the usual Euclidean space $\mathbb{R}^3$ will be discussed in details in Section II. In the thermodynamic limit, the properties of the model depend solely upon the coupling parameter $\Gamma = \beta q^2/a_i$ ($\beta = 1/kT$, k Boltzmann constant, T temperature, and a_i the ionic radius defined by $4\pi\rho a_i^3/3 = 1$, where $\rho = N/\Lambda$ is the number density of ions) and upon the reduced screening parameter $\alpha^* = \alpha a_i$.

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In this paper we report Monte Carlo (MC) simulations of the YOCP in the canonical ensemble and within hyperspherical boundary conditions. The idea of using the two dimensional (2D) surface of an ordinary sphere to perform numerical simulations of a 2D fluid phase can be traced back to a paper by J. P. Hansen *et al.* devoted to a study of the electron gaz at the surface of liquid Helium.[9] Subsequently, the same idea was used to study the crystalization of the 2D one-component plasma (OCP) (with log interactions).[10] The generalization of the method to 3D systems, implying the use of a 4D sphere (in short a hypersphere), is due to Caillol and Levesque.[11] The method was subsequently used to study various models pertaining to the field of chemical physics such that ionic and polar fluids,[11] colloidal suspensions,[12, 13] and even the Lennard–Jones fluid.[14] More recently the method was applied to the OCP ($\alpha^* = 0$)[15] and we consider here the case of the YOCP ($\alpha^* \neq 0$).

The expression of the Yukawa potential on the hypersphere $\mathscr{S}^3$—i.e., the Green's function of the Helmholtz equation in $\mathscr{S}^3$—is derived in the companion paper (hereafter refered as I) as well as all the formal expressions (configurational energy, formal lower bounds, etc.) which are required for simulations performed in this geometry. The aim of our simulations was to provide input data for a model of equation of state (EOS) of the Hydrogen and Deuterium plasmas which is discussed elsewhere.[16, 17] Previous numerical studies by Hamaguchi *et al.*[1–4] did not cover a sufficiently large domain of (α^*, Γ) in view of these applications. In order to apply our results to the physical conditions of the last Nova experiments of shock compressed liquid deuterium,[18] it appeared necessary to perform MC simulations for $0.1 \leqslant \Gamma \leqslant 100$ and for $0.1 \leqslant \alpha^* \leqslant 6$.

Our paper is organized as follows. In Section II we present the Hamiltonian of the YOCP in $\mathbb{R}^3$ and propose a new method for a precise determination of the excess free energy. In Section III we give briefly some technical details on the numerical procedure used in our MC calculations. The datas are presented anal discussed in Section IV and the conclusions are drawn in Section V.

II. THE MODEL

A. Yukawa Systems in $\mathbb{R}^3$

Before considering the complicated case of the YOCP within hyperspherical boundary conditions, let us first discuss the usual Euclidean case. We therefore consider a neutral classical plasma made of N identical point charges q (ions) immersed in a uniform neutralizing background (electrons) of volume Λ and charge density $-qp$. The configurational energy of the

model has been given by Hubbard and Slattery[19] for cubico-periodical geometries. In our case, we need a slight generalization of their expression which reads as

$$V^{\mathbb{R}^3}(1,\ldots,N) = \frac{1}{2}\sum_{i=1}^{N}\sum_{i\neq j}^{N} v_\alpha(r_{ij}) - \sum_{i=1}^{N}\int_{\Lambda} d^3\mathbf{r}\,\rho v_\alpha(|\mathbf{r}-\mathbf{r}_i|) + \frac{1}{2}\int_{\Lambda^2} d^3\mathbf{r}\,d^3\mathbf{r}'\,\rho^2 v_\alpha(|\mathbf{r}-\mathbf{r}'|) + N\mathscr{E} \tag{2.1}$$

In Eq. (2.1), $v_\alpha(r)$ denotes the effective interactions between the ions due to the polarizable background of electrons. The r.h.s. of Eq. (2.1) includes the particle–particle, particle–background, and background–background interactions as well as an additional constant $N\mathscr{E}$ which fixes the zero of energy, the expression of which reads as

$$\mathscr{E} = \frac{1}{2}\lim_{r\to 0}\left[v_\alpha(r) - \frac{q^2}{r}\right] \tag{2.2}$$

Note that if the term $N\mathscr{E}$ is included in $V^{\mathbb{R}^3}(1,\ldots,N)$, the zero of energy is defined with respect to the self-energy of a bare (Coulomb) charge rather than that of an "effective" charge (i.e., a charge in the presence of the background). Of course, both self-energies diverge but their difference should remain a finite quantity for any reasonable model.

The use of effective pair interactions to describe the influence of the background is obviously a crude approximation. We make a still cruder approximation by assuming that $v_\alpha(r)$ is a Yukawa potential

$$v_\alpha(r) = q^2\frac{\exp(-\alpha r)}{r} \tag{2.3}$$

Mathematically $v_\alpha(r)$ is the Green's function of Helmoltz equation in $\mathbb{R}^3$ which vanishes at infinity, i.e.,

$$(\Delta - \alpha^2)\,v_\alpha(r) = -4\pi q^2\delta^3(\mathbf{r}) \tag{2.4}$$

The case $\alpha = 0$ corresponds to the usual OCP and, in the case $\alpha \neq 0$, we deal with the YOCP. In the YOCP the influence of the background is; taken into account in the frame of the linear response theory by assuming that its dielectric constant has the simple expression

$$\varepsilon(\mathbf{k}) = 1 + \alpha^2/\mathbf{k}^2 \tag{2.5}$$

which can be obtained when the electrons are described in the frame of either the linearised Debye–Huckel theory (LDH) or the Thomas–Fermi theory.[20] In the former case we deal with a hot dilute electron gaz whereas, in the latter, we deal with a cold and dense quantum gaz of electrons. The explicit dependance of the screening parameter $\alpha \equiv \alpha(\rho, T)$ upon the density ρ and the temperature T depends obviously on the model under consideration. Note by passing, that, for Yukawa effective interactions, the constant $\mathscr{E}$ is indeed a finite quantity, $\mathscr{E} = -q^2\alpha/2$. More realistic dielectric functions $\varepsilon(\mathbf{k})$ have been considered in the literature,[21–24] however it is shown in ref. 17 that the Yukawa potential is a sufficiently good approximation in many cases.[17]

For sufficiently large systems ($\Lambda \to \infty$) the thermodynamic and structural properties of the YOCP depend on the sole dimensionless parameters (α^*, Γ) and the expression (2.1) $\beta V^{\mathbb{R}^3}(1,..., N)$ can be rewritten as

$$\beta V^{\mathbb{R}^3}(1,..., N) = \frac{\Gamma}{2} \sum_{i=1}^{N} \sum_{i \neq j}^{N} \frac{\exp(-\alpha^* r_{ij})}{r_{ij}} - N\left(\frac{3\Gamma}{2\alpha^{*2}} + \frac{\Gamma\alpha^*}{2}\right) \tag{2.6}$$

where the interparticle distances r_{ij} are measured in the unit of the ionic radius a_i.

Let us denote $f = \beta F/N$ the excess reduced free energy per particle ($F \equiv$ free energy) of the model. Its derivatives with respect to α^* and Γ, are easily expressed as thermal averages of pair potentials:

$$f_{\alpha^*} = \frac{\partial f(\alpha^*, \Gamma)}{\partial \alpha^*} = \left(\frac{3}{\alpha^{*3}} - \frac{1}{2}\right)\Gamma + \frac{\Gamma}{2N}\left\langle \sum_{i=1}^{N} \sum_{i \neq j} \exp(-\alpha^* r_{ij}) \right\rangle \tag{2.7}$$

$$f_{\Gamma} = \frac{\partial f(\alpha^*, \Gamma)}{\partial \Gamma} = \frac{1}{2N}\left\langle \sum_{i=1}^{N} \sum_{i \neq j}^{N} \frac{\exp(-\alpha^* r_{ij})}{r_{ij}} \right\rangle - \frac{3}{2\alpha^{*2}} - \frac{\alpha^*}{2} \tag{2.8}$$

where $\langle \cdots \rangle$ denotes a canonical average. Applying the second Stillinger–Lovett sum rule[25] to the case of the OCP ($\alpha^* = 0$), one easily shows that

$$\lim_{\alpha^* \to 0} f_{\alpha^*} = 0 \tag{2.9}$$

and, using the ideal gaz limit (valid for totally screened interactions) one also obtains

$$\lim_{\alpha^* \to +\infty} f_{\alpha^*} = -\Gamma/2 \tag{2.10}$$

Moreover, in the general case where the effective screening parameter α^* of the considered model depends on both the temperature and the density, the

excess internal energy u and the excess pressure p are respectively given by

$$\beta u(\alpha^*, \Gamma) = \beta \left(\frac{\partial f(\alpha^*, \Gamma)}{\partial \beta} \right) = \Gamma \left(\frac{\partial f(\alpha^*, \Gamma)}{\partial \Gamma} \right) + \beta \left(\frac{\partial \alpha^*}{\partial \beta} \right) \left(\frac{\partial f(\alpha^*, \Gamma)}{\partial \alpha^*} \right) \tag{2.11}$$

and

$$\begin{aligned} \frac{\beta p(\alpha^*, \Gamma)}{\rho} &= 1 + \rho \left(\frac{\partial f(\alpha^*, \Gamma)}{\partial \rho} \right) \\ &= 1 + \frac{\Gamma}{3} \left(\frac{\partial f(\alpha^*, \Gamma)}{\partial \Gamma} \right) + \rho \left(\frac{\partial \alpha^*}{\partial \rho} \right) \left(\frac{\partial f(\alpha^*, \Gamma)}{\partial \alpha^*} \right) \end{aligned} \tag{2.12}$$

B. Free Energy

In order to calculate the excess free energy, we devised an original method which consists in integrating f_{α^*} with respect to α^* rather than f_Γ with respect to Γ as usual.[26] We therefore write

$$f(\alpha^*, \Gamma) = f(\alpha^* = 0, \Gamma) + \int_0^{\alpha^*} \frac{\partial f(\alpha_1^*, \Gamma)}{\partial \alpha_1^*} \, d\alpha_1^* \tag{2.13}$$

which can be conveniently rewritten as

$$f(\alpha^*, \Gamma) = f_{\mathrm{OCP}}(\Gamma) + f_{\mathrm{YUK}}(\alpha^*, \Gamma) \tag{2.14}$$

where $f_{\mathrm{OCP}}(\Gamma)$ is the excess free energy of the OCP which is known with a high degree of precision from previous numerical studies.[15, 26]

Note that the numerical determination of f_{α^*} in an actual MC simulations is conveniently obtained from Eq. (2.7). From the knowledge of f and of its derivatives with respect to Γ and α^*, and given the density and temperature dependence of the screening parameter, all thermodynamic quantities are determined using Eqs. (2.11), (2.12). Thus, the knowledge of the density and temperature dependence of the screening parameter is sufficient to determine self-consistently all thermodynamical properties, taking advantage of the very precise MC data for f_{OCP}.[15, 26]

III. NUMERICAL DETAILS

A. Expressions of the Thermodynamic Quantities on the Hypersphere

The hypersphere $\mathscr{S}^3$ of center O and radius R is the set of points $\mathbf{OM} = (x, y, z, t)$ of $\mathbb{R}^4$ which satisfy the relation $x^2 + y^2 + z^2 + t^2 = R^2$.

$\mathscr{S}^3$ is a 3D non-Euclidean closed manifold of $\mathbb{R}^4$ of positive curvature which is homogeneous and isotropic albeit finite and thus well adapted for the numerical simulation of a fluid phase. Its volume is $\Lambda = 2\pi^2 R^3$. The Green's function of Helmholtz equation can be obtained analytically in $\mathscr{S}^3$ which makes the geometry appealing for numerical simulations of screened Coulomb systems. The configurational energy of a YOCP made of N ions of charge q confined in $\mathscr{S}^3$ was derived in paper I. It reads

$$\beta V^{\mathscr{S}^3}(1,\ldots,N) = \frac{\beta q^2}{2} \sum_{i=1}^{N} \sum_{j \neq i} v_\alpha^{\mathscr{S}^3}(\psi_{ij}) + N\beta\mathscr{A} \tag{3.1}$$

where the pair potential $v_\alpha^{\mathscr{S}^3}(\psi)$ ($\psi \in [0, \pi]$) is given by

$$\begin{aligned} v_\alpha^{\mathscr{S}^3}(\psi) &= \frac{1}{R} \frac{\sinh \omega(\pi - \psi)}{\sin \psi \sinh \omega\psi} - \frac{4\pi}{\alpha^2 \Lambda}, \qquad \text{for} \quad \alpha R \geqslant 1 \\ &= \frac{1}{R} \frac{\sin \omega(\pi - \psi)}{\sin \psi \sin \omega\psi} - \frac{4\pi}{\alpha^2 \Lambda}, \qquad \text{for} \quad \alpha R \leqslant 1 \end{aligned} \tag{3.2}$$

where $\omega = (|\alpha^2 R^2 - 1|)^{1/2}$. The pair potential $v_\alpha^{\mathscr{S}^3}(\psi)$ is isotropic and depends on the sole geodesic length $R\psi$. The geodesic distance between two ions located respectively at points M_i and M_j of $\mathscr{S}^3$ being obviously given by

$$d_{ij} = R\psi_{ij} = R \arccos\left(\frac{\mathbf{OM}_i \cdot \mathbf{OM}_j}{R^2}\right) \tag{3.3}$$

The constant $\mathscr{A}$ in Eq. (3.1) which fixes the zero of energy is the sum of two contributions

$$\beta\mathscr{A} = \beta\mathscr{A}_{\mathrm{OCP}} + \beta\delta\mathscr{A} \tag{3.4}$$

the former being the constant which fixes the zero of energy of the OCP ($\alpha = 0$) in $\mathscr{S}^3$ i.e.,[15]

$$\begin{aligned} \beta\mathscr{A}_{\mathrm{OCP}} &= -\frac{9}{10}\Gamma - \frac{3\Gamma}{4\pi R^*} + \frac{\Gamma}{2R^* d(\psi_0)} \left[\frac{3}{2} + \sin^2(\psi_0) - \frac{\psi_0 \sin^2(\psi_0)}{d(\psi_0)}\right] \\ d(\psi_0) &= \psi_0 - \sin(\psi_0)\cos(\psi_0) \end{aligned} \tag{3.5}$$

where $\psi_0 = a^{\mathscr{S}^3}/R$, $R^* = R/a^{\mathscr{S}^3}$ (reduced radius of $\mathscr{S}^3$) and $\Gamma = \beta q^2/a^{\mathscr{S}^3}$ (coupling parameter), $a^{\mathscr{S}^3}$ being the ionic radius in $\mathscr{S}^3$ defined as the solution of the following transcendental equation

$$2\pi\rho R^3 d(\psi_0) = 1$$

The second contribution $\delta\mathscr{A}$ to $\mathscr{A}$ vanishes when $\alpha = 0$ and reads as

$$\begin{aligned}\beta\delta\mathscr{A} &= \frac{\Gamma}{2}\left[\frac{3}{2\pi R^*} - \frac{\omega\coth\omega\pi}{R^*} - \frac{4\pi}{\alpha^{*2}\Lambda^*}\right], \qquad \text{for} \quad \alpha R \geqslant 1 \\ &= \frac{\Gamma}{2}\left[\frac{3}{2\pi R^*} - \frac{\omega\coth\omega\pi}{R^*} - \frac{4\pi}{\alpha^{*2}\Lambda^*}\right], \qquad \text{for} \quad \alpha R \leqslant 1 \end{aligned} \tag{3.6}$$

where $\alpha^* \equiv \alpha a^{\mathscr{S}^3}$ is the reduced screening parameter and $\Lambda^* \equiv \Lambda/(a^{\mathscr{S}^3})^3$ the reduced volume.

One easily establishes that, in the canonical ensemble, the derivatives of the reduced excess free energy f with respect to Γ and α^* are given by the following expressions

$$\Gamma(\partial f/\partial\Gamma) = \frac{1}{N}\langle \beta V^{\mathscr{S}^3}(1,\ldots,N)\rangle \tag{3.7a}$$

$$(\partial f/\partial\alpha^*) = \frac{1}{N}\langle \beta W^{\mathscr{S}^3}(1,\ldots,N)\rangle \tag{3.7b}$$

which should be compared with their Euclidean counterparts (2.7) and (2.8). In Eq. (3.7a)

$$\beta W^{\mathscr{S}^3}(1,\ldots,N) = N(\partial\beta\mathscr{A}/\partial\alpha^*) - \frac{\Gamma}{2}\sum_{i=1}^{N}\sum_{j\neq i} w_\alpha^{\mathscr{S}^3}(\psi_{ij}) \tag{3.8}$$

The pair function $w_\alpha^{\mathscr{S}^3}(\psi)$ which enters Eq. (3.8) is given by

$$\begin{aligned} w_\alpha^{\mathscr{S}^3}(\psi) &= \frac{\pi\alpha R}{\omega}\frac{\cosh\omega\pi\sinh\omega(\pi-\psi)}{\sin\psi\sinh^2\omega\pi} \\ &\quad - \frac{\alpha R}{\omega}\frac{(\pi-\psi)\cosh\omega(\pi-\psi)}{\sin\psi\sinh\omega\psi} - \frac{4}{\pi\alpha^3R^3} \qquad (\alpha R \geqslant 1) \\ &= \frac{\pi\alpha R}{\omega}\frac{\cos\omega\pi\sin\omega(\pi-\psi)}{\sin\psi\sin^2\omega\pi} \\ &\quad - \frac{\alpha R}{\omega}\frac{(\pi-\psi)\cos\omega(\pi-\psi)}{\sin\psi\sin\omega\psi} - \frac{4}{\pi\alpha^3R^3} \qquad (\alpha R \leqslant 1) \end{aligned} \tag{3.9}$$

and the additive constant $\partial\beta\mathscr{A}/\partial\alpha^* \equiv \partial\beta\,\delta\mathscr{A}/\partial\alpha^*$ by

$$\partial\beta\,\delta\mathscr{A}/\partial\alpha^* = \frac{\Gamma}{2}\left[\frac{4}{\pi\alpha^3R^3} + \frac{\alpha R}{\omega}\left(\frac{\omega\pi}{\sinh^2\omega\pi} - \coth\omega\pi\right)\right] \qquad (\alpha R \geqslant 1)$$

$$= \frac{\Gamma}{2}\left[\frac{4}{\pi\alpha^3R^3} + \frac{\alpha R}{\omega}\left(\frac{\omega\pi}{\sin^2\omega\pi} - \cot\omega\pi\right)\right] \qquad (\alpha R \leqslant 1) \qquad (3.10)$$

B. Numerical Evaluation of the Pair Functions

The way of performing MC simulations in $\mathscr{S}^3$ was described in many previous papers[11, 15] and we discuss here only the numerical procedure retained to compute the thermal averages (3.7). The pair functions $v_\alpha^{\mathscr{S}^3}(\psi)$ and $w_\alpha^{\mathscr{S}^3}(\psi)$ which enter Eqs. (3.7) can been obtained with a high degree of accuracy by simple interpolation schemes. Let us denote by $f(\psi)$ either $(v_\alpha^{\mathscr{S}^3}(\psi) - v_\alpha^{\mathscr{S}^3}(\pi))$ or $(w_\alpha^{\mathscr{S}^3}(\psi) - w_\alpha^{\mathscr{S}^3}(\pi))$. In both cases $f(\psi)$ is a non negative decreasing function of ψ for $\psi \in [0, \pi]$. In fact, the variable $X \equiv (1 - \cos\psi)$ is more suitable for numerical purposes since, for a pair of particles, the determination of $X_{ij} = 1. - \mathbf{OM}_i \cdot \mathbf{OM}_j/R^2$ is convenient and requires only 8 floating point operations. We have evaluated $f(X)$ according to the following scheme

- $0 \leqslant \psi \leqslant \psi_1$: direct calculation of $f(X)$.
- $\psi_1 \leqslant \psi \leqslant \psi_2$: Hermite quadratic interpolation of $f(X)$.[27]
- $\psi_2 \leqslant \psi \leqslant \pi$: linear interpolation of $f(X)$.

For a given number N of particles and a given screening parameter α^*, it is always possible to choose an interpolation interval $\delta X = 2/n_{\text{grid}}$ ($n_{\text{grid}} \equiv$ number of points of the grid of interpolation), and a couple of angles ψ_1 and ψ_2 such that the relative precision on $f(X)$ is smaller than some ascribed value p, $\forall X \in (0, 2]$. This point was discussed in detail in the case of the OCP.[15] As also discussed at length in the same reference, a relative precision of p on the pair function $f(X)$ ensures that the numerical relative error on either $\beta\langle V^{\mathscr{S}^3}(1,..., N)/N\rangle$ or $\beta\langle W^{\mathscr{S}^3}(1,..., N)/N\rangle$ is also smaller than p. Obviously p must be chosen several orders of magnitude smaller than the expected statistical errors which originate from the MC procedure. In all our simulations $n_{\text{grid}} = 30000$ and ψ_1 and ψ_2 where chosen such that $p = 10^{-8}$. Moreover, for high α^* and large system sizes, the function $f(\psi)$ vanishes at large ψ's and was set to zero in this range in order to speed up the calculations with no consequences on the precision of the MC data.

IV. NUMERICAL RESULTS

In a recent theory of the EOS of the totally ionized Hydrogen (or Deuterium) plasma the authors propose a model for the screening of ion–ion interactions which involves an effective Yukawa potential characterized by an effective screening parameter $\alpha^*(\rho, T)$ which depends explicitly on the density and temperature of the plasma.[16, 17] The thermodynamic conditions (ρ, T) of the last Nova experiments of shock compressed liquid Deuterium,[18] correspond, within this theoretical scheme, to values of Γ in the range $[0, 100]$ and of α^* in the range $[0, 6]$. None of the existing data provided by the litterature[1–4, 21–24] cover these ranges of parameters. This state of affairs motivated the present numerical study. In order to cover all thermodynamical conditions of the Nova experiments it thus appeared necessary to perform MC simulations for $\Gamma = 0.1$, 0.5, 1.0, 2.0, 5.0, 10.0, 20.0, 40.0, 60.0, 80.0, 100.0 and for $\alpha^* = 0.1$, 0.2, 0.4, 0.6, 0.8, 1.0, 1.4, 2.0, 2.5, 3.0, 3.5, 4.0, 5.0, 6.0.

In all our simulations we considered systems of $N = 600$ particles and, for each state (Γ, α^*), $M = 60 \times 10^6$ configurations were generated after equilibrium. The relative statistical uncertainties on f_{α^*} and f_Γ which were calculated by a standard block analysis procedure,[28] are typically $\sim 5 \times 10^{-4}$ or less. Previous numerical studies on the OCP[15] have shown that the thermodynamic limit is certainly riot reached for a system of $N = 600$ ions. This is of course also the case for the YOCP considered here. A finite size scaling study was performed for some states (Γ, α^*) and revealed that the differences between the values of f_{α^*} and f_Γ calculated at the thermodynamical limit and the values obtained for $N = 600$ are slightly larger than the statistical errors reported in the tables. Although possible in principle, a more systematic study would require a prohibitive demand in CPU time.

The numerical results for f_{α^*} and f_Γ are reported in Tables I to IV. Tables I and III correspond to the lowest values of Γ for f_{α^*} and f_Γ respectively. Table II and IV give the same results for the highest values of Γ. These results are also displayed in Fig. 1 (for f_{α^*}) and in Fig. 2 (for f_Γ). For both functions the MC results are plotted versus α^*, for different values of Γ. On Fig. 1, we observe the convergence of f_{α^*} towards its asymptotic limits (2.9) and (2.10) for all values of Γ.

We performed an analytical representation of f_{α^*},[17] in the spirit of previous parametrizations of the OCP.[26] Our fit, which represents the MC datas for values of the coupling parameters in the ranges $0.1 \leqslant \Gamma \leqslant 100$ and $0.1 \leqslant \alpha^* \leqslant 6.0$, correctly reproduces the limiting laws (2.9) and (2.10). It reads as

$$f_{\alpha^*} = -a(\alpha) \times \Gamma - b_1(\alpha)\, \Gamma^{1/3} - b_2(\alpha)\, \Gamma^{-1/3} - b_3(\alpha) \ln \Gamma - b_4(\alpha) \qquad (4.1)$$

Table I. MC Data for $(\partial f/\partial \alpha^*)$ for Various Values of the Screening Parameter α^* and Low Values of the Coupling Parameter Γ [a]

α^*	$\Gamma=0.1$	$\Gamma=0.5$	$\Gamma=1$	$\Gamma=2$	$\Gamma=3$	$\Gamma=5$
0.1	−0.014079(07)	−0.038378(08)	−0.058185(11)	−0.089772(16)	−0.117574(19)	−0.168859(31)
0.2	−0.028869(10)	−0.072870(26)	−0.112460(31)	−0.175154(42)	−0.230675(27)	−0.332921(65)
0.4	−0.043386(17)	−0.126541(34)	−0.203192(55)	−0.327025(50)	−0.436757(62)	−0.639579(63)
0.6	−0.048774(15)	−0.163291(29)	−0.273335(48)	−0.454300(55)	−0.615888(67)	−0.915069(70)
0.8	−0.050444(10)	−0.188220(26)	−0.326871(65)	−0.559771(74)	−0.769492(99)	−1.16018(13)
1.0	−0.049901(16)	−0.205037(16)	−0.367078(25)	−0.645942(84)	−0.899809(98)	−1.37464(17)
1.4	−0.050101(10)	−0.224544(13)	−0.416579(13)	−0.770397(52)	−1.09697(11)	−1.71621(10)
2.0	−0.050021(5)	−0.237232(10)	−0.458414(23)	−0.875265(45)	−1.274377(45)	−2.04700(9)
2.5	−0.049980(3)	−0.241976(7)	−0.473786(9)	−0.919438(18)	−1.355564(38)	−2.206580(77)
3.0	−0.049963(2)	−0.244589(5)	−0.482437(10)	−0.946689(12)	−1.402317(25)	−2.303074(48)
3.5	−0.049960(1)	−0.246158(5)	−0.487201(06)	−0.962402(12)	−1.432652(18)	−2.362639(29)
4.0	−0.049960(1)	−0.247148(4)	−0.490891(7)	−0.972883(10)	−1.450698(11)	−2.400764(14)
5.0	−0.049967(00)	−0.248293(2)	−0.494570(3)	−0.984506(6)	−1.471738(5)	−2.444269(17)
6.0	−0.049981(00)	−0.248885(1)	−0.496577(2)	−0.990022(6)	−1.482356(4)	−2.465331(8)

[a] In all simulations $N=600$. The numbers into brackets which correspond to *one* standard deviation are the statistical uncertainties on the last digits.

Table II. MC Data for $(\partial f/\partial \alpha^*)$ for Various Values of the Screening Parameter α^* and High Values of the Coupling Parameter Γ [a]

α^*	$\Gamma=10$	$\Gamma=20$	$\Gamma=40$	$\Gamma=60$	$\Gamma=80$	$\Gamma=100$
0.1	−0.287361(27)	−0.511486(31)	−0.944902(35)	−1.37156(6)	−1.794920(98)	−2.21626(8)
0.2	−0.569485(47)	−1.016995(87)	−1.882455(84)	−2.73400(16)	−3.57904(21)	−4.42068(23)
0.4	−1.10843(26)	−1.997104(99)	−3.71545(17)	−5.40623(18)	−7.08495(26)	−8.75547(30)
0.6	−1.60987(21)	−2.92606(16)	−5.47339(15)	−7.98061(25)	−10.46863(48)	−12.9469(5)
0.8	−2.06938(11)	−3.79474(15)	−7.13638(22)	−10.42583(30)	−13.69144(63)	−16.9425(5)
1.0	−2.48458(15)	−4.59544(24)	−8.68764(16)	−12.71774(35)	−16.71805(51)	−20.7011(7)
1.4	−3.17852(15)	−5.97625(24)	−11.41260(19)	−16.77166(24)	−22.09301(36)	−27.3930(4)
2.0	−3.90301(20)	−7.49238(15)	−14.50783(34)	−21.43794(29)	−28.32747(33)	−35.1912(5)
2.5	−4.27683(16)	−8.31833(16)	−16.26212(23)	−24.12849(53)	−31.95622(44)	−39.7605(3)
3.0	−4.51197(15)	−8.85657(17)	−17.43849(15)	−25.95887(18)	−34.44685(19)	−42.9159(2)
3.5	−4.660517(48)	−9.203643(65)	−18.21202(28)	−27.17396(21)	−36.11224(22)	−45.0351(3)
4.0	−4.756485(70)	−9.429742(63)	−18.72091(8)	−27.97870(12)	−37.21913(15)	−46.4485(3)
5.0	−4.863746(30)	−9.683686(51)	−19.29401(7)	−28.88743(7)	−38.47203(12)	−48.0506(1)
6.0	−4.916625(10)	−9.808111(14)	−19.57474(3)	−29.33191(3)l	−39.084351(45)	−48.83373(9)

[a] In all simulations $N=600$. The numbers into brackets which correspond to *one* standard deviation are the statistical uncertainties on the last digits.

Table III. MC Data for $(\partial f/\partial \Gamma)$ for Various Values of the Screening Parameter α^* and Low Values of the Coupling Parameter Γ [a]

α^*	$\Gamma=0.1$	$\Gamma=0.5$	$\Gamma=1$	$\Gamma=2$	$\Gamma=3$	$\Gamma=5$
0.1	−0.025078(09)	−0.234484(26)	−0.569993(36)	−1.320380(89)	−2.11502(10)	−3.76136(24)
0.2	−0.022806(11)	−0.237856(32)	−0.574891(39)	−1.329089(84)	−2.127020(75)	−3.77994(20)
0.4	−0.027921(11)	−0.250883(25)	−0.595852(54)	−1.363581(71)	−2.17501(11)	−3.85356(12)
0.6	−0.035211(11)	−0.271683(33)	−0.629442(46)	−1.420260(71)	−2.253640(92)	−3.97551(11)
0.8	−0.043770(08)	−0.298901(18)	−0.674670(67)	−1.497767(86)	−2.361701(88)	−4.14246(14)
1.0	−0.053547(11)	−0.331462(24)	−0.730088(38)	−1.594062(89)	−2.49639(10)	−4.35253(17)
1.4	−0.072554(11)	−0.407510(18)	−0.867261(19)	−1.834961(45)	−2.83772(11)	−4.88787(11)
2.0	−0.101831(06)	−0.537569(14)	−1.107244(19)	−2.284408(48)	−3.485319(66)	−5.919369(89)
2.5	−0.126514(06)	−0.653201(10)	−1.329419(16)	−2.710238(26)	−4.105787(50)	−6.923470(89)
3.0	−0.151300(04)	−0.772083(11)	−1.561305(18)	−3.159931(13)	−4.771561(37)	−8.009956(64)
3.5	−0.176135(03)	−0.892898(14)	−1.799528(11)	−3.626597(25)	−5.462184(24)	−9.148379(43)
4.0	−0.201013(03)	−1.014927(12)	−2.040238(15)	−4.102366(17)	−6.171883(18)	−10.319776(24)
5.0	−0.250842(02)	−1.260976(09)	−2.528973(08)	−5.071527(16)	−7.619368(11)	−12.718892(28)
6.0	−0.300718(04)	−1.508574(05)	−3.021952(06)	−6.053875(17)	−9.088413(12)	−15.160941(19)

[a] In all simulations $N=600$. The numbers into brackets which correspond to *one* standard deviation are the statistical uncertainties on the last digits.

Table IV. MC Data for $(\partial f/\partial \Gamma)$ for Various Values of the Screening Parameter α^* and High Values of the Coupling Parameter Γ [a]

α^*	$\Gamma=10$	$\Gamma=20$	$\Gamma=40$	$\Gamma=60$	$\Gamma=80$	$\Gamma=100$
0.1	−8.01012(23)	−16.6977(4)	−34.30821(54)	−52.0346(10)	−69.8191(16)	−87.6414(11)
0.2	−8.04426(16)	−16.7633(5)	−34.43546(59)	−52.2262(11)	−70.0745(17)	−87.9539(20)
0.4	−8.18187(23)	−17.0258(4)	−34.94766(58)	−52.98780(69)	−71.0821(10)	−89.2139(12)
0.6	−8.40798(24)	−17.4597(3)	−35.79303(48)	−54.24226(69)	−72.7481(13)	−91.2842(16)
0.8	−8.72032(24)	−18.0584(3)	−36.95988(49)	−55.97561(63)	−75.0449(15)	−94.1475(09)
1.0	−9.11417(19)	−18.8141(3)	−38.43394(31)	−58.16379(57)	−77.94784(87)	−97.7659(12)
1.4	−10.12314(19)	−20.7549(3)	−42.22329(19)	−63.79378(36)	−85.41589(48)	−107.06738(48)
2.0	−12.09045(19)	−24.5647(2)	−49.68276(34)	−74.88883(31)	−100.13694(37)	−125.41188(52)
2.5	−14.03323(15)	−28.3560(2)	−57.13663(22)	−85.98961(54)	−114.87827(39)	−143.78807(36)
3.0	−16.15694(15)	−32.5291(2)	−65.37653(13)	−98.27958(15)	−131.21092(18)	−164.15836(23)
3.5	−18.39852(6)	−36.95738(7)	−74.15211(27)	−111.38914(21)	−148.64682(23)	−185.91740(21)
4.0	−20.71616(9)	−41.55394(7)	−83.28667(9)	−125.0510(1)	−166.83064(16)	−208.61975(23)
5.0	−25.48596(4)	−51.04540(7)	−102.19834(8)	−153.36877(8)	−204.54777(14)	−255.73225(11)
6.0	−30.35307(2)	−60.75390(3)	−121.57671(5)	−182.41038(4)	−243.24908(05)	−304.09091(11)

[a] In all simulations $N=600$. The numbers into brackets which correspond to *one* standard deviation are the statistical uncertainties on the last digits.

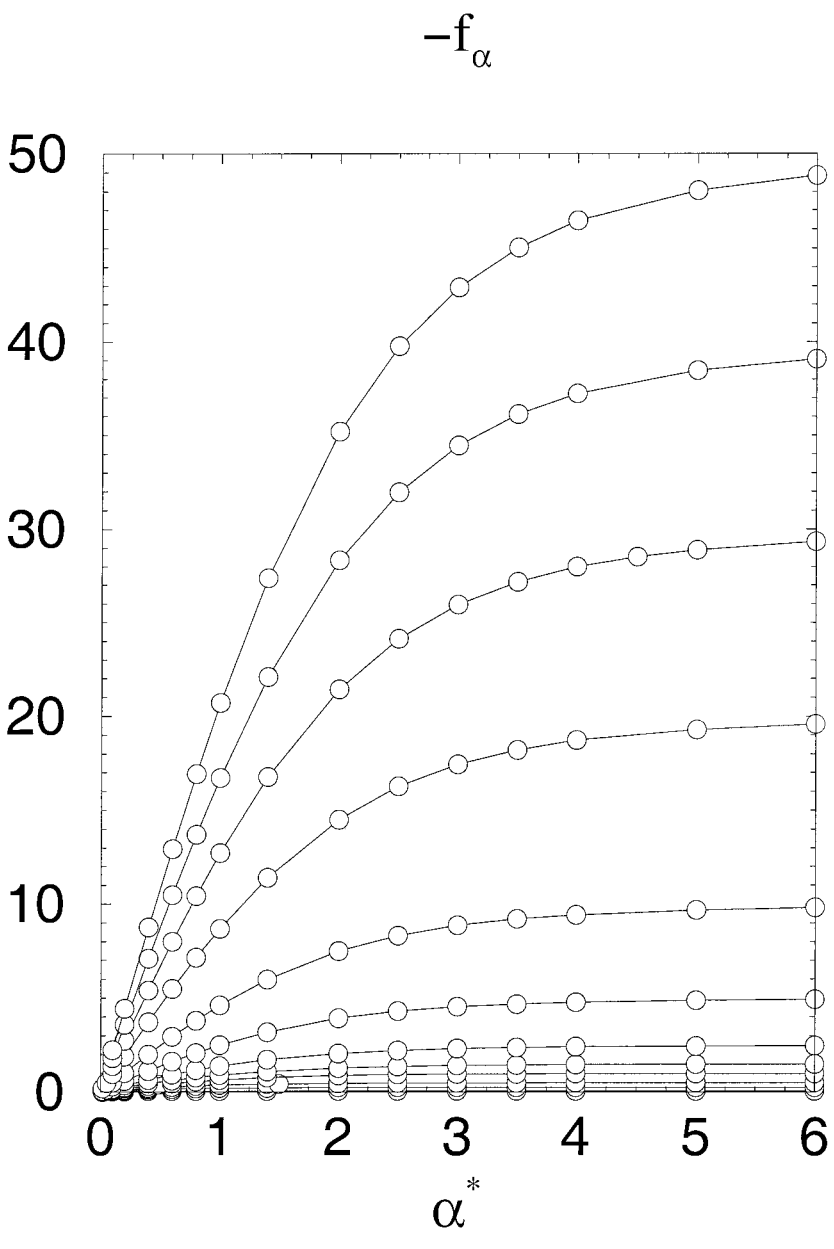

Fig. 1. $-(\partial f/\partial\alpha)$ as a function of α^* for various values of Γ. From bottom to top $\Gamma = 0.1, 0.5, 1, 2, 3, 5, 10, 20, 40, 60, 80, 100$. The error bars on the displayed results, which correspond to one standard deviation, are smaller than the symbol sizes. The solid lines are the result of the fit (4.1).

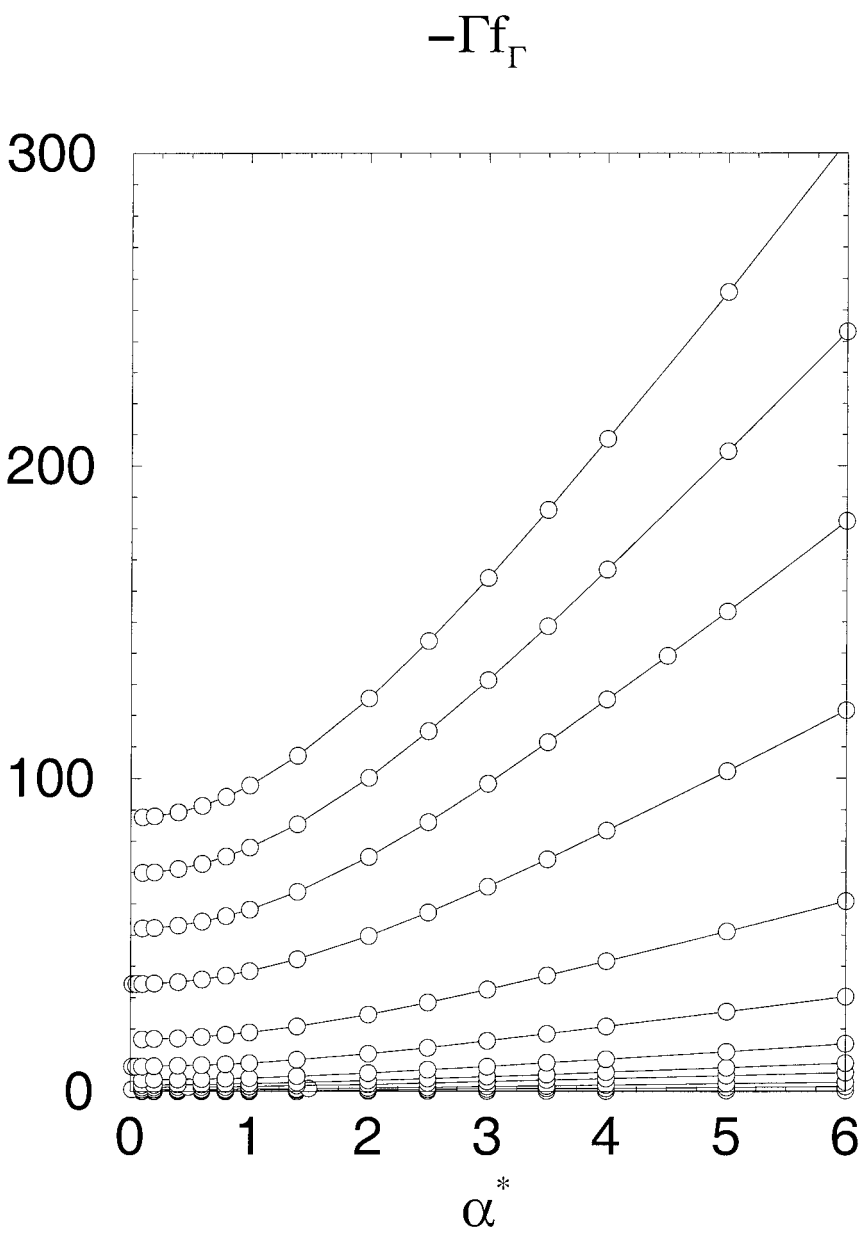

Fig. 2. $-\Gamma(\partial f/\partial\Gamma)$ as a function of α^* for various values of Γ. From bottom to top $\Gamma = 0.1, 0.5, 1, 2, 3, 5, 10, 20, 40, 60, 80, 100$. The error bars on the displayed results, which correspond to one standard deviation, are smaller than the symbol sizes. The solid lines are the result of the fit (4.1).

Table V. Coefficients of the Fit (4.1), (4.2)

i	a_i	$b_{1,i}$	$b_{2,i}$	$b_{3,i}$	$b_{4,i}$
0	0.895518	0.255048	0.227173	0.193532	0.039849
1	0.493174	0.113309	−2.15654	−1.29895	8.11973
2		−0.222818	10.0333	7.92197	−34.6655
3		3.47069	−5.37412	−4.53558	5.26751
4		0.002995	0.445334	−0.003648	−0.62045
5		1.568751	1.604841	1.740061	1.44286

where the coefficients are given by

$$a(\alpha) = \tfrac{1}{2}(1 - \exp(-a_0\alpha)(1 + a_1\alpha)) \tag{4.2}$$

$$b_i(\alpha) = (1 - \exp - b_{i,0}\alpha)(1 + b_{i,1}\alpha + b_{i,2}\alpha^2 + b_{i,3}\alpha^3 + b_{i,4}\alpha^4)\exp(-b_{i,5}\alpha)$$

The numerical values of the constants which enter Eq. (4.2) are given in Table V. The free energy f is then obtained from Eq. (2.13). Note that, with this method, we take advantage of the very precise results already known for the OCP.[15, 26] We stress again that the knowledge of f_{α^*} and of the screening parameter $\alpha^*(\rho, T)$ is sufficient to determine self-consistently all the thermodynamical properties of the system (see Eqs. (2.11) and (2.12)).

V. CONCLUSION

In this work, we have determined the excess free energy of the YOCP for a wide range of values of Γ and α^* by means of MC simulations on a hypersphere. Due to the large number of considered states a finite size scaling study of the results, such as the one performed recently for the OCP in ref. 15 was impossible. However as discussed in Section IV the values for f obtained for $N = 600$ differ only but slightly from their thermodynamic limit and have been used extensively in a recent study of the Deuterium EOS.[16] The results reported in this paper can be used to determine the energy and the pressure of any model of plasma with an arbitrary dependence of the screening parameter α^* upon the density and the temperature as discussed in Section IV. Besides this study of the thermodynamic properties of the YOCP we have also computed the microfield distribution functions, these results are discussed elsewhere.[29]

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