ON THE LINEAR BEHAVIOR OF THE SCREENING POTENTIAL IN HIGH-DENSITY OCP PLASMAS

DO XUAN HOI*, TRAN THI NGOC LAM**

ABSTRACT

Based on the importance of the short range order effect of the plasmas OCP, which is expressed through the damped oscillations of the pair correlation function g(r), we carry out elaborate examinations of the location r_{max} as well as of the amplitude g_{max} of its first maximum for various values of the screening parameter and put forward for the first time the analytical formulae for these data. The linear variation of the screening potential for some interionic distance can be therefore explained thoroughly by considering the relation between this first maximum and the screening potential. Especially, using this accurate fit of g_{max} established for dense OCP plasmas, we expand it to the region of weakly correlated ones and point out the value Γ_C of the correlation parameter for which there exists the onset of the short range order effect. This value is very close to ones proposed in other works.

Keywords: plasmas OCP, screening potential, pair correlation function, Monte Carlo simulations, linear behavior, threshold of short range order effect, analytical formula.

TÓM TẮT

Về dạng biến thiên tuyến tính của thế màn chắn trong plasma OCP mật độ cao

Dựa trên các dao động tắt dần của hàm tương quan cặp, biểu thị của hiệu ứng trật tự địa phương, các tác giả bài báo khảo sát chi tiết vị trí và độ lớn g_{max} của cực đại đầu tiên của hàm này tương ứng với các giá trị khác nhau của tham số màn chắn và đề nghị các biểu thức giải tích cho các dữ liệu này. Từ đó, sự biến thiên tuyến tính của thế màn chắn đối với một khoảng cách nhất định của khoảng cách liên ion được giải thích rõ ràng. Đặc biệt, dựa trên các biểu thức chính xác của g_{max} thiết lập cho plasma đậm đặc, chúng tôi đã nới rộng cho vùng plasma loãng và tìm được giá trị ngưỡng Γ_C của hiệu ứng trật tự địa phương. Giá trị tìm thấy rất gần với các kết quả đề nghị trong những công trình trước đây.

Từ khóa: plasma OCP, thế màn chắn, hàm tương quan cặp, mô phỏng Monte Carlo, dạng tuyến tính, ngưỡng của hiệu ứng trật tự địa phương, công thức giải tích.

1. Introduction

The screening potential $H(R)$ expresses the influence of the medium on the interaction between two particles. In an OCP (One-Component-Plasma) plasma, this potential is computed from the potential of mean force:

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$$V(R) = \frac{(Ze)^2}{R} - H(R) \tag{1}$$

where the first quantity on the right hand side is the Coulomb potential between two ions of charge *Ze*, separated by *R*. The potential *H*(*R*) plays an important role in the study of some astrophysical objects of high density such as brown dwarfs and neutron stars, as well as in the laboratory plasmas [9]. The denser the plasmas are, the more evident the effect of the screening is. Especially, as shown by many works related to the field, at short distance between the two particle, the screening reduces considerably the Coulomb repulsion and consequently leads to an increase of nuclear reaction rate [11]. The numerical data of this screening potential are obtained from the Monte Carlo (MC) simulations carried out for the pair distribution function:

$$g(R) = \exp\left[-\beta V(R)\right] \tag{2}$$

where $\beta = \frac{1}{kT}$; *k* and *T* are respectively the Boltzmann constant and the plasmas temperature. The model OCP, shown to be useful in the study of plasmas, is characterized by the correlation parameter $\Gamma = \frac{(Ze)^2}{akT}$ measuring the importance of Coulomb interaction with respect to the kinetic energy. In this formula, *a* is ion sphere radius.

In this work, we shall systematically use the MC data for OCP provided by DeWitt *et al* [4]. Those data are considered to be accurate enough in comparing with the other simulations recently performed. Just like the pioneer works [1], the numerical data clearly show the oscillations of the function *g*(*r*), signature of short range order effect. (See Fig 1.) In studying in detail the variation of *g*(*r*) and of the screening *H*(*r*), the scientific community have been wondered at a particular behavior of *H*(*r*). That is, in some range of the distance *r*, this function can be expressed as [3]:

$$H(r) = C_0 - C_1 r\,, \tag{3}$$

with the empirical relation:

$$C_0 = 2\sqrt{C_1}\,. \tag{4}$$

where *r* is defined as the reduced interionic distance: $r = \frac{R}{a}$.

In fact, as pointed out in some of our previous works [8, 10], this linear behavior can be explained by considering the damped oscillation of the function *g*(*r*), and the location as well as the magnitude of these peaks should be used as important data to determine the general expression for the screening potential *H*(*r*).

In this work, after a detailed consideration of the MC numerical values of the function $g(r)$, we shall suggest the analytical expressions for the first maxima of $g(r)$: their location, and the amplitude of the short range order effect. The linear behavior of $H(r)$ is examined elaborately and the coefficients C_0 and C_1 in (3) will be expressed in analytical form. Especially, we shall prove that the threshold value of this effect can be deduced on base of the accuracy of these formulae.

2. Location and amplitude of short range order effect

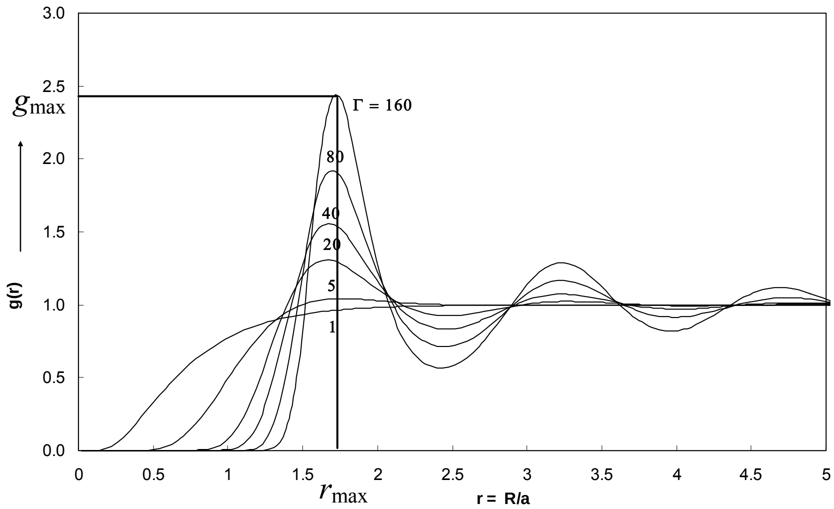


Fig.1 Damped oscillations of the function g(r) for various values of Γ. Location (r_{max}, g_{max}) of the first maximum of g(r)

As indicated above, the determination of the first maximum of the function $g(r)$ plays a primordial role in computing the screening potential. For this reason, we have carried out the study of these parameters [10]. The numerical values for $r_{\max}$ and $g_{\max} \equiv g(r_{\max})$ are shown in Table 1 and 2. They are also compared with some previous results [7]. We notice that although the difference is considerable only for small values of Γ, this discrepancy is meaningful for our computation of the threshold value of Γ.

Table 1. Numerical values of positions of first maximum of the function $g(r)$. *The new values of r_{max} are shown in the second column. In the third and fifth columns, those values are found in [6] and [7]. An important difference between the numerical values can be remarked for Γ = 5.*

Γ	$r_{\max}$	$r_{\max 99}$	$\Delta r_{\max 99}$	$r_{\max 02}$	$\Delta r_{\max 02}$
3.17	1.920425				
5	1.765152	1.750305	-14.85×10^{-3}	1.7756	10.45×10^{-3}
10	1.670331	1.67398	3.65×10^{-3}	1.6745	4.17×10^{-3}
20	1.664608	1.66218	-2.43×10^{-3}	1.6615	-3.11×10^{-3}

40	1.676169	1.67525	$- 0.92\times10^{-3}$	1.6745	-1.67×10^{-3}
80	1.698999	1.69793	$- 1.07\times10^{-3}$	1.6985	-0.50×10^{-3}
160	1.724468	1.72443	$- 0.04\times10^{-3}$	1.7245	0.03×10^{-3}

Table 2. Numerical values of amplitudes of first maximum of the function *g*(*r*). *We can pay attention to the good agreement between the new values of g_{max} and the older ones [7]. However, in this work, the value of g_{max} for Γ = 3.17 is found for the first time, which will play a crucial role for the determination of the threshold of the short range effect.*

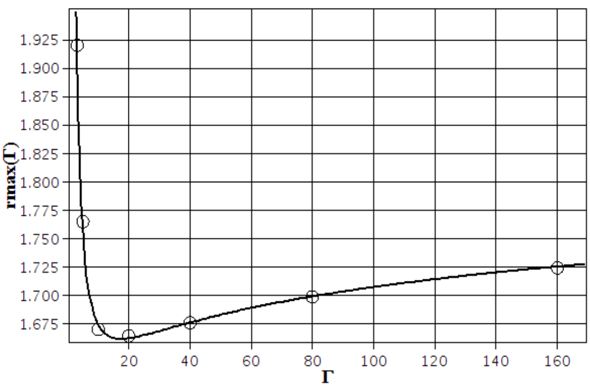
Γ	g_{max}	g_{max02}	Δg_{max02}
3.17	1.010794		
5	1.041320	1.0418	-0.48×10^{-3}
10	1.138460	1.1398	-1.34×10^{-3}
20	1.306735	1.3046	2.14×10^{-3}
40	1.558768	1.5581	0.67×10^{-3}
80	1.922923	1.9232	-0.28×10^{-3}
160	2.438075	2.4409	-2.83×10^{-3}

Based on those results, we propose these analytical formulae for r_{max} and $g_{max} \equiv g(r_{max})$:

$$r_{max}(\Gamma) = 1.51876 + 0.04047\ln(\Gamma) + 2.02961\times 0.22099^{ln(\Gamma)} \quad (5)$$

$$g_{max}(\Gamma) = 2.89645 - 1.92686e^{-0.00887\Gamma} \quad (6)$$

The variation of these functions with respect to the screening parameter Γ is found to be regular (Fig. 2) and at the same time, the discrepancy between these functions and their numerical values is only about 0.1% as we can see in Table 3, which can be considered to be satisfied if we recall that the error for the MC simulations is of the same order.



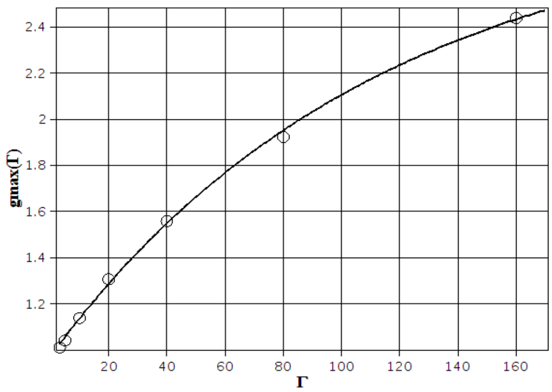


Fig 2. ***The variation of r_{max} and of g_{max} with respect to the variable Γ. The minimum of r_{max} is noticed for Γ = 20. On the contrary, the function g_{max} does not prove any***

Table 3. **Comparison of numerical values of location and amplitude of the first maximum of the function *g*(*r*).** *The accuracy of the formulae (5) and (6) is clearly shown by considering the errors* Δr_{max} *and* Δg_{max} *between (5) and (6) and their values given in Tables 1 and 2 .*

Γ	$r_{\max}$	$\Delta r_{\max}$	$g_{\max}$	$\Delta g_{\max}$
3.17	1.921078	-0.03 %	1.010794	-1.21 %
5	1.762634	0.14 %	1.041320	-1.14 %
10	1.674719	-0.26 %	1.138460	0.46 %
20	1.662043	0.15 %	1.306735	1.82 %
40	1.675791	0.02 %	1.558768	0.86 %
80	1.69882	0.01%	1.922923	-1.37 %
160	1.725107	-0.04%	2.438075	0.29 %

3. Linear function of the screening potential

As demonstrated in a previous work [5], the linear behavior of the screening potential can be explained by introducing a parameter $\delta = \frac{\ln g_{\max}}{\Gamma}$ that expresses the difference between this potential $H(r)$ and the Coulomb potential at point $r_{\max}$. Indeed, from (1) and (2), the radial distribution function can be written:

$$g(r) = \exp\left[-\Gamma\left(\frac{1}{r} - H(r)\right)\right] \tag{7}$$

or alternatively:

$$H(r) = \frac{1}{r} + \frac{1}{\Gamma}\ln g(r)\,. \tag{8}$$

By remarking that at the first maximum of $g(r)$, we have: $\left.\frac{dg}{dr}\right|_{r=r_{\max}} = 0$, and by using a Taylor expansion at point $r_{\max}$, we obtain:

$$H(r) = \frac{1}{r_{\max}} + \frac{1}{\Gamma}\ln g_{\max} + \left[-\frac{1}{r_{\max}^2} + \left(\frac{1}{\Gamma}\frac{dg/dr}{g}\right)_{r=r_{\max}}\right](r - r_{\max}) + \ldots$$

Keeping only the terms in r, we can write:

$$H(r) = \frac{2}{r_{\max}} + \frac{1}{\Gamma}\ln g_{\max} - \frac{r}{r_{\max}^2}\,.$$

At this point, the below expression for the screening potential:

$$H(r) = C_0 - C_1 r \quad (9)$$

where:

$$C_0 = \frac{2}{r_{\max}} + \delta$$

and

$$C_1 = \frac{1}{r_{\max}^2}.$$

give us an idea of its linear variation in some range of the interionic distance *r* and of the relation:

$$C_0 = 2\sqrt{C_1} + \delta. \quad (10)$$

Note that the empirical relation (3), which has caught the attention of many physicists in the field, can be obtained only with very small magnitude of the parameter *δ*. Of course, this relation is valid only for some value of *r*, and note that the range of r depends on the density of plasmas as well, as we can see in Table 4.

In order to clarify the dependence of δ on the correlation parameter Γ, we have made a detailed study of the numerical results from the MC simulations and put forward this analytical expression:

$$\delta(\Gamma) = \left(2.53271 - 0.38942 \ln\Gamma - 3.77684 \times 0.78284^{\Gamma}\right) \times 10^{-2} \quad (11)$$

which is valid for $\Gamma \in [3.17, 160]$.

(to compare with $\delta(\Gamma) = \left(0.544 - 0.401 \ln\frac{\Gamma}{160}\right) \times 10^{-2}, \quad \Gamma \in [140, 200]$ given in [5]).

Its variation is shown on the Fig. 3, where we can recognize its sensitiveness to the parameter Γ.

We introduce here two analytical formulae for the coefficients C_0 and C_1, which prove a high consistence with their numerical values [10]:

$$C_0(\Gamma) = 1.27779 - 0.02024 \times \ln(\Gamma) - 0.70857 \times 0.67608^{\Gamma} \quad (12)$$

$$C_1(\Gamma) = 0.39001 - 0.00971 \times \ln(\Gamma) - 0.36624 \times 0.67731^{\Gamma} \quad (13)$$

In order to have a clearer view of the relation of C_0, C_1 and the amplitude of the sort range order effect δ, we present the Fig. 4, where the close agreement between C_0 and $2\sqrt{C_1} + \delta$ can be recognized.

Table 4. About the linear behavior of the screening potential. *We present in the columns 2 and 3 the extent of interionic distance from r_{min} to r_{max} where the linear behavior of the screening potential can be applied. The numerical values of the coefficients C_0 and C_1 are shown in columns 4 and 5. We can compare the values of $C_0 - 2\sqrt{C_1}$ and those of δ given in columns 6 and 7.*

Γ	r_{min}	r_{max}	C_0	C_1	$100(C_0-2\sqrt{C_1})$	100δ
3.17	1.67686	2.16398	1.04868	0.27191	0.57802	0.3387
5	1.52668	2.00361	1.14761	0.32325	1.050842	0.8098
10	1.42761	1.91305	1.21216	0.35809	1.534757	1.2968
20	1.41665	1.89572	1.22108	0.36269	1.660501	1.3377
40	1.44477	1.90756	1.204	0.35452	1.316836	1.1097
80	1.47385	1.92414	1.18672	0.34614	1.004672	0.817
160	1.50329	1.94564	1.17557	0.34113	0.744329	0.5570

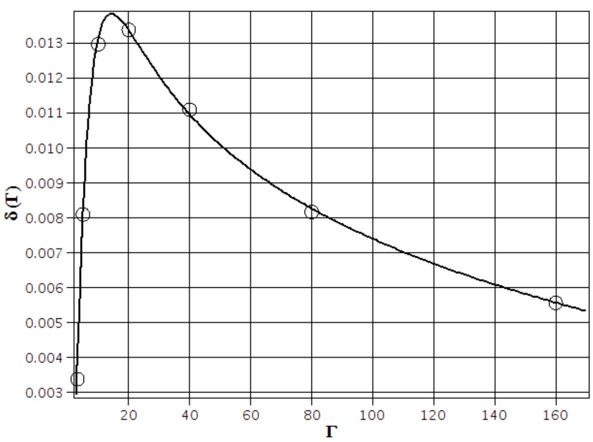


Fig 3. *The rapid variation of δ(Γ) with small value of Γ shows that the linear expression for H(r) is more accurate for dense plasmas.*

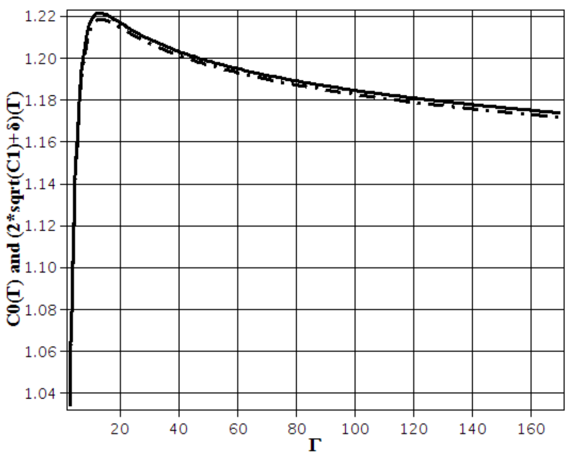


Fig 4. *The comparison of the coefficients C_0, C_1 and the amplitude of short range order effect δ.*

4. Threshold of short range order effect

The value of the correlation parameter Γ for which the function $g(r)$ begin to express the oscillation is still unspecified. According to some authors, this value Γ_C can be evaluated in the range from 0.99 to 1.8206 [2]. In one of our works [6], by considering the properties of fluid plasmas, we deduced $\Gamma_C = 1.75$. Recently, based on the same method, Nguyễn Thị Thanh Thảo [12] proposed the value $\Gamma_C = 1.8006$, which is closer to the one offered by F. D. Rio and H. E. De Witt. In this work, with the formula (6) obtained by a elaborate examination of MC simulations data, we can have the value of Γ_C by equalizing (6) to unity, in reminding that the maximum value of the pair distribution function $g(r)$ for weakly correlated plasmas can only be unit:

$$g_{max}(\Gamma \leq \Gamma_C) = 2.89645 - 1.92686e^{-0.00887\Gamma} = 1\,.$$

This equality is based on the assumption that the formula (6), established for dense plasmas, can be expanded to the less correlated ones.

Solving this equation gives us the wanted value: $\Gamma_C = 1.79$ [10], also close to the numerical value of F. D. Rio and H. E. De Witt and of Nguyễn Thị Thanh Thảo. This result proves also that the formula (6) is quite adequate to describe the first maximum $g_{\max}$ of the function $g(r)$.

5. Conclusion

By determining the location $r_{\max}$ as well as the magnitude of the first maximum $g_{\max}$ of the pair correlation function $g(r)$, we propose a clear explanation of the linear behavior of the screening potential, one of the remarkable properties of dense plasmas. For a more elaborate study of this range of plasmas, we offer at the same time the analytical formulae for $r_{\max}$ and $g_{\max}$, which will be useful for applying the method of parametrization of the effect of short range order effect to the computation of the screening potential in dense and fluid plasmas. One direct application of this analytical form of the amplitude $g_{\max}$ is the deduction of the value Γ_C, at which the onset of the oscillation of $g(r)$ is established. This value is found to be conform to other results.

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(Received: 30/5/2011; Accepted: 05/8/2011)