ANALYTIC EXPRESSIONS CHARACTERIZING THE DAMPED OSCILLATION OF THE RADIAL DISTRIBUTION FUNCTION IN HIGH DENSITY OCP PLASMAS

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ABSTRACT

In this work, we show an elaborate study of the damped variation of the radial distribution function g(r) with respect to the interionic distance r. The analytic expressions of the positions as well as the values of the five extrema of g(r) are proposed for the first time, based on the most accurate numerical Monte Carlo simulation data for OCP system. The damping behavior of the function g(r) is also presented so that one can use it to determine the extrema of g(r) for crystallized plasmas with extremely high value of correlation parameter. These important results contribute to precise the screening potential in OCP plasmas by using the method of parametrization of the short range order effect.

Keywords: OCP system, Monte Carlo simulations, radial distribution function, damped oscillation, screening potential, analytical formula, short range order effect.

TÓM TẮT

Các biểu thức giải tích đặc trưng cho dao động tắt dần của hàm phân bố xuyên tâm trong plasma OCP mật độ cao

Trong công trình này, chúng tôi trình bày một khảo sát công phu sự dao động tắt dần của hàm phân bố xuyên tâm g(r) đối với khoảng cách liên ion r. Lần đầu tiên, các biểu thức giải tích cho các vị trí cũng như giá trị của năm cực trị của g(r) được đề nghị, dựa trên các dữ liệu mô phỏng Monte Carlo chính xác nhất cho tới hiện nay cho hệ plasma OCP. Dáng điệu tắt dần của hàm g(r) cũng được trình bày để ta có thể sử dụng với mục đích xác định các cực trị của g(r) cho plasma kết tinh với giá trị rất lớn của tham số tương liên. Các kết quả quan trọng này đóng góp cho việc xác định thế màn chắn trong plasma OCP bằng phương pháp tham số hóa hiệu ứng trật tự địa phương.

Từ khóa: Hệ plasma OCP, mô phỏng Monte Carlo, hàm phân bố xuyên tâm, dao động tắt dần, thế màn chắn, hệ thức giải tích, hiệu ứng trật tự địa phương.

1. Introduction

In very early works on computational simulations for an OCP (One Component Plasma) system [4, 9, 10], the damped oscillation of the radial distribution function (RDF) $g(r)$ has been pointed out. This particular property, especially for the ultradense OCP, can be considered as the signature of the short range order effect that appears in a plasma system [7, 11]. These authors have also given some characteristics of the function $g(r)$ such as their position and value of the first maximum. But, with the purpose of using this oscillatory variation to determine the screening potential (SP) in

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an OCP, one needs a more detailed study on this function $g(r)$. In this paper, we carry out a systematic consideration of this behavior of $g(r)$ by studying carefully the position and the value of each extremum. We also try to introduce analytic expressions for these quantities. This will show clearly the damping oscillation of $g(r)$ for ultradense plasmas, and then, can give us the way to find out the other extremum for weakly correlated ones. Besides, an extension of this study will be useful for the determination of the extrema of $g(r)$ for the crystallization of extremely dense OCP system. One of important applications of this study is related to the calculation of the SP using the procedure of the parameterization of the short range effect in OCP.

As in several works on the OCP, we shall use the correlation parameter:

$$\Gamma = \frac{(\mathrm{Ze})^2}{\mathrm{akT}} \tag{1}$$

to indicate the importance of the average Coulomb interaction $\frac{(Ze)^2}{a}$ between charged particles with respect to the random motion energy kT, the distance a being defined as the ion sphere radius. The RDF $g(r)$, that characterizes the probability of finding a particle at a distance of r away from a given reference particle, is related to the SP $H(R)$ by:

$$\mathrm{g(R = ar) = exp} - \frac{1}{\mathrm{kT}}\left[\frac{(\mathrm{Ze})^2}{\mathrm{R}} - \mathrm{H(R)}\right] \tag{2}$$

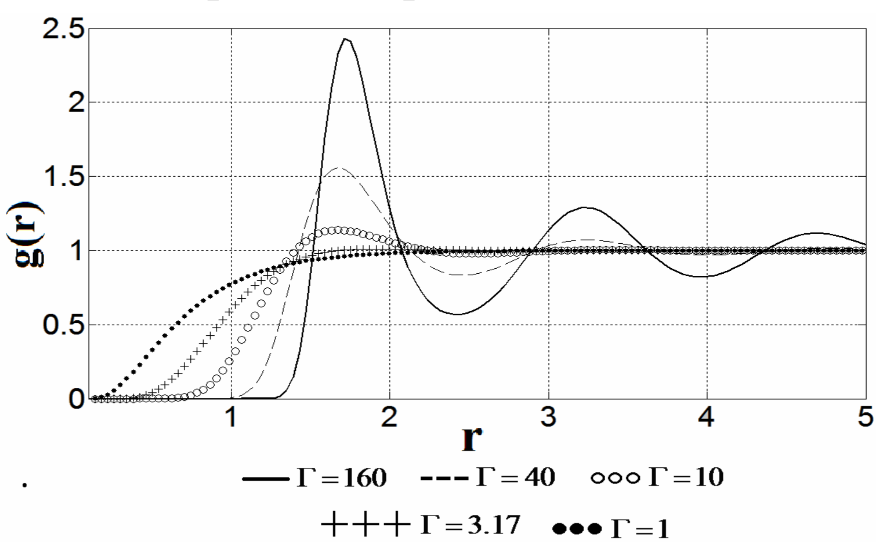

Fig 1. *The damped oscillation of g(r) for Γ > 1 and the uniform variation of g(r) for Γ = 1. Data taken from [5].*

2. Analytic expressions for extrema of the radial distribution function *g*(*r*)

One of the first observations of the variation of the RDF *g*(*r*) with respect to the distance *r* is that the maxima g_{max} are more pronounced when the plasmas are denser, i.e. when the quantity Γ takes more important values. For this reason, it is not obvious to obtain these maxima for dilute plasmas. And then, one can see that the position of each extremum depends clearly on the value of Γ.

In Figure 1, we recognize the rapid rate of damping of *g*(*r*) for important value of Γ. On the contrary, this function takes an increasing behavior for $\Gamma \leq 1$. The threshold value of Γ for which the oscillation of *g*(*r*) occurs has been considered in several works (see [3], for example). The values of the first maximum g_{max1} of *g*(*r*) and its location have appeared in various works for the reason that, considered as ones of the parameters characterizing the short range order effect, they contribute to the determination of the SP *H*(*r*) of the OCP, especially to the rate of enhancement of nuclear fusion [11]. Before giving general expressions for those values, we present in Table 1 and Table 2 some characteristics of the first extrema of the RDF *g*(*r*) [1].

Table 1. *Values of the first maxima of g(r) and comparison with other works*

Γ	g_{max}	$10^3 \Delta g_{max}$			
		[11]	[6]	[9]	[4]
3.17	1.010515		0.21		
5	1.041063	0.51	- 0.02		- 1.4
10	1.138506	0.68	- 0.11	3.5	12.1
20	1.306216	- 0.41	0.02	- 3.8	- 11.1
40	1.559343	- 0.59	- 0.33	- 0.7	- 6.1
80	1.921606	0.46	1.04	1.6	
160	2.443333	- 5.71	- 5.58	1.4	

We can see the excellent agreement between the data of this work with that of [11] and [6]. The more recent data of [9] corresponds better to our work than those of [4]. Notice that in this paper as well as in [6], we can reach the g_{max} fot dilute plasmas whereas in the others [4, 9, 11], those data are hardly obtained. For the location of the first maximum, a discrepancy of about some of thousandth between our calculation and that of [6, 11] is noticed.

Table 2. *Values of the position of the first maxima of g(r) and comparison with other works*

Γ	r_{max}	$10^3 \Delta r_{max}$	
		[11]	[6]
3.17	1.912349		- 27.34
5	1.764928	14.62	8.72
10	1.677864	3.88	4.59
20	1.666712	4.53	4.80
40	1.679623	4.37	4.18
80	1.702373	4.44	4.35
160	1.728841	4.41	4.30

With the purpose to generalize these values for other quantities of Γ, we carry out a careful examination of almost all extrema and their locations up to $r = 8.41$ and obtain the data given in Table 3 for Γ = 160 for example. We propose at the same time these analytic expressions:

$$g_{max160}\left(r_{max}\right) = 13.34e^{-1.355r_{max}} + 1.207e^{-0.0217r_{max}}, \quad (3)$$

$$g_{min160}\left(r_{min}\right) = 1.015\,e^{-0.002026r_{min}} - 1.74\,e^{-0.5651r_{min}}. \quad (4)$$

The errors committed between (3) and (4) and the numerical data in Table 3 is below 5‰.

Table 3. *Values for the first five maxima and the first five minima as well as their positions for Γ = 160*

Extremum	r_{max}	g_{max}	r_{min}	g_{min}
1	1.728841	2.443333	2.422479	0.566960
2	3.234256	1.290842	3.961061	0.820554
3	4.693018	1.116727	5.455641	0.924393
4	6.183251	1.052984	6.928998	0.964934
5	7.666125	1.024805	8.407899	0.982606

With the formulae (3) and (4), one sees more clearly the strong damping behavior of *g*(*r*) for Γ = 160, as presented in Figure 2.

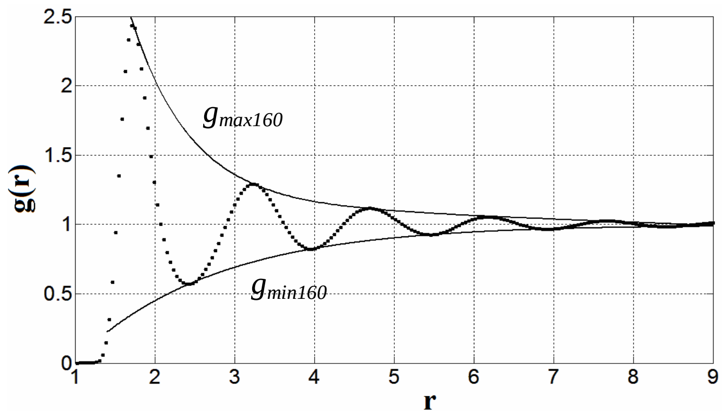

Fig 2. *The boundaries of the maxima and the minima expressed by (3) and (4) for Γ = 160. The black circles are MC data taken from [5].*

We recognize that the work becomes more difficult with more dilute plasmas, the reason is that the extrema are less pronounced for these media. This characteristic can be seen in Figure 3 where the variation of $g(r)$ is more weekly damped for $\Gamma = 20$.

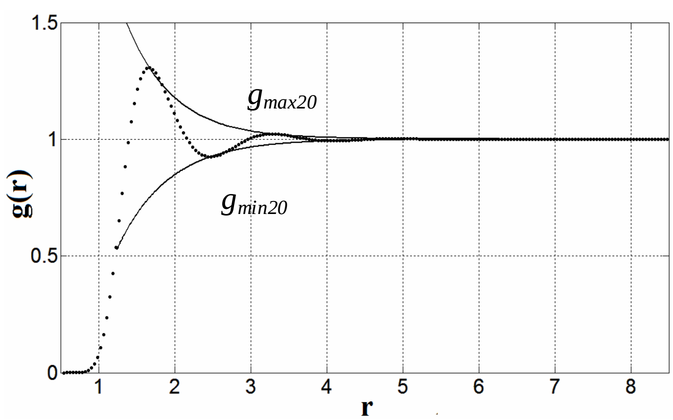

Fig 3. *The damping behavior for Γ = 20 is more slowly in comparison with Γ = 160*

Anyway, in some case, one needs the value of first maximum and its position of $g(r)$ for some particular value of the parameter Γ, for example, the one corresponding to the crystallization of ultradense plasmas, phenomenon announced by physicists working in this field [2, 8]. To this aim, after analyzing the MC data, we put forward these formulae for each available value of Γ:

$$g_{\max 80} = 7.439\,e^{-1.261 r_{\max}} + 1.067 e^{-0.007804 r_{\max}} \tag{5a}$$

$$g_{\max 40} = 5.486\,e^{-1.371 r_{\max}} + 1.014 e^{-0.001796 r_{\max}} \tag{5b}$$

$$g_{\max 20} = 4.69\,e^{-1.64 r_{\max}} + 1.002 e^{-0.000196 r_{\max}} \tag{5c}$$

Note the missing formulae for dilute plasmas with Γ < 20. Based on (5a, b, and c), we obtain

$$g_{max}\left(r_{max}\right) = A_1 e^{A_2 r_{max}} + A_3 e^{A_4 r_{max}} \quad (6)$$

with the coefficients A_1, A_2, A_3, A_4 given in Table 4.

***Table 4**. Values of coefficients used in (6)*

Γ	A_1	A_2	A_3	A_4
20	4.69	- 1.64	1.002	- 0.000196
40	5.486	- 1.371	1.014	- 0.001796
80	7.439	- 1.261	1.067	- 0.007804
160	13.34	- 1.355	1.207	- 0.0217

For extended uses, we generalize values of these coefficients for arbitrary value of Γ:

$$A_1(\Gamma) = 4.1\times10^{-7}\Gamma^3 + 9.302\times10^{-5}\Gamma^2 + 0.03307\Gamma + 3.988 \quad (7a)$$

$$A_2(\Gamma) = 1.04\times10^{-6}\Gamma^3 - 3.24\times10^{-4}\Gamma^2 + 0.02998\Gamma - 2.118 \quad (7b)$$

$$A_3(\Gamma) = -6.101\times10^{-8}\Gamma^3 + 2.063\times10^{-5}\Gamma^2 - 4.667\times10^{-4}\Gamma + 1.004 \quad (7c)$$

$$A_4(\Gamma) = 6.958\times10^{-9}\Gamma^3 - 2.144\times10^{-6}\Gamma^2 + 2.917\times10^{-5}\Gamma + 2.267\times10^{-5} \quad (7d)$$

The variation of the coefficients A_i (i = 1,…, 4) is shown in Figure 4. Their continuity with respect to Γ is acceptable. The magnitude of the discrepancy between (6) and the MC data is shown to be satisfying and although the fitting is made principally for Γ = 20; 40; 80; 160, the difference between (6) and other value of g_{max} is below 10%.

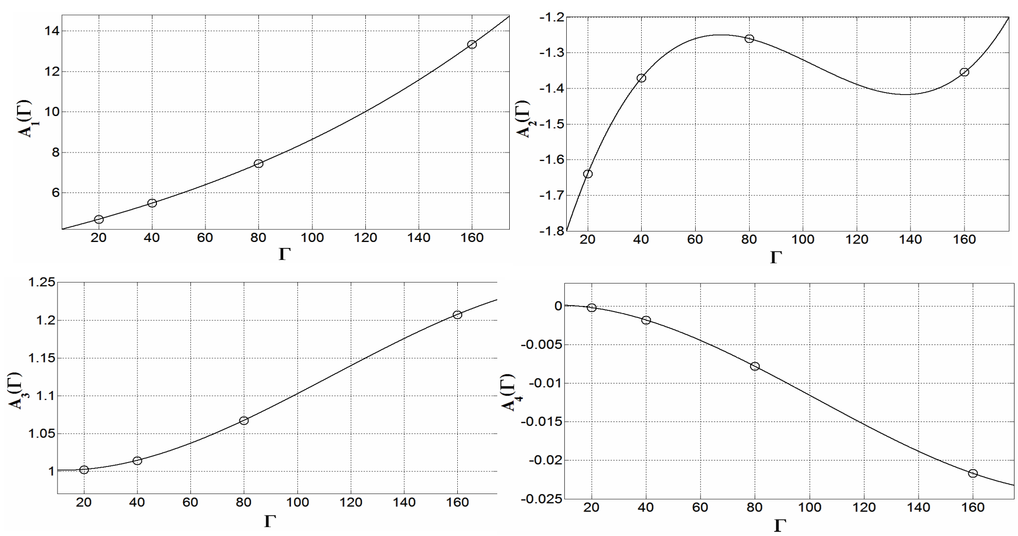

***Fig 4.** Continuity of the variation of A_i with respect to Γ*

For all other minima corresponding to any value of Γ, we can use:

$$g_{min}\left(r\right) = B_1 e^{B_2 r_{min}} + B_3 e^{B_4 r_{min}} \quad (8)$$

In Table 5, we find the numerical values for (8).

Table 5. *Values of coefficients used in (8)*

Γ	B_1	B_2	B_3	B_4
20	0.9995	0.000059	- 3.008	- 1.493
40	0.997	0.000337	- 2.542	- 1.112
80	0.9901	0.000978	- 2.098	- 0.8217
160	1.015	- 0.002026	- 1.74	- 0.5651

The same procedure as for the first maxima gives us, for the first minima:

$$B_1(\Gamma) = 3.445\times10^{-8}\Gamma^3 - 5.615\times10^{-6}\Gamma^2 + 1.154\times10^{-4}\Gamma + 0.992 \quad (9a)$$

$$B_2(\Gamma) = -3.442\times10^{-9}\Gamma^3 + 5.173\times10^{-7}\Gamma^2 - 7.5\times10^{-6}\Gamma + 2.962\times10^{-5} \quad (9b)$$

$$B_3(\Gamma) = 1.058\times10^{-6}\Gamma^3 - 3.515\times10^{-4}\Gamma^2 + 0.04143\Gamma - 3.704 \quad (9c)$$

$$B_4(\Gamma) = 1.163\times10^{-6}\Gamma^3 - 3.593\times10^{-4}\Gamma^2 + 0.03735\Gamma - 2.106 \quad (9d)$$

In order to verify the accuracy of these expressions, we compare (9a, b, c, and d) with MC numerical values. The result obtained persuades us of their exactness.

3. Applications

As mentioned above, once the behavior of the damped oscillation of the radial distribution function $g(r)$ determined by analytic formulae, we can deduce important features of an OCP system.

One of these applications is to obtain the extrema and their locations of $g(r)$ for the critical value of the correlation parameter Γ = 172 where there occurs the crystallization. We carry out the computation based on (6) and (8) and compare with other work, [2] for example. The result is shown in Table 6; the discrepancy between those works is very small.

Table 6. *Comparison between this paper's result and [2]*

Γ = 172		[2]	Error
r_{max}	1.736069	1.731661	0.44%
r_{min}	2.410080	2.419429	1.14%
g_{max}	2.518926	2.507493	0.93%
g_{min}	0.554900	0.548937	0.60%

Another result of (6) and (8) is more interesting when one deduces the numerical value of the coefficients of the Widom polynomial expressing the SP for an OCP:

$$H(r) = h_0 - h_1 r^2 + h_2 r^4 - ... + (-1)^i h_i r^{2i} + ... = \sum_{i\geq 0} (-1)^i h_i r^{2i} \quad (10)$$

In [11], the method of parametrization of the short range order effect has been developed to acquire the value of h_i in (10) up to a twelfth degree polynomial with the use of the first maximum of $g(r)$. Now, with the result obtained not only for this first maximum but for the first minimum as well, we perform a quite sophisticated computation and get numerical values for the coefficients in (10), which are shown in Table 7. Note that the interionic distance r is now extended to $r \in [0, 3.32]$ instead of $r \in [0, 2.72]$ as in [11], so that one can cover the two first extrema of $g(r)$. It is then obvious that the discrepancy between $g(r)$ calculated from (10) and MC data becomes more important.

Table 7. *Numerical values of Widom expansion (10) for the SP in an OCP system*

Γ	h_0	h_1	$10^2 h_2$	$10^3 h_3$	$10^4 h_4$	$10^5 h_5$	$10^6 h_6$
5	1.083262	0.263559	4.275705	3.971224	2.009625	0.476669	0.030929
10	1.095227	0.258669	3.790193	2.946100	1.184026	0.273517	0.053194
20	1.091730	0.251688	3.459187	2.352153	0.715228	0.115005	0.035180
40	1.087180	0.251160	3.483051	2.401442	0.714631	0.058619	0.004863
80	1.078876	0.250138	3.587753	2.795153	1.324634	0.517681	0.140892
160	1.073900	0.250019	3.594238	2.646076	0.913759	0.146974	0.028895

4. Conclusion

This is the first time the damping oscillation behavior of the radial distribution function $g(r)$ for an OCP plasma system is studied in such a systematic method. The result for five extrema of this function as well as their locations is presented in form of analytic formulae, which can produce important information of the extrema of $g(r)$ for any value of the correlation parameter and then favors considerably computational works on computers. Moreover, the short range order effect that appears in this physical system is parametrized covering the first maximum and the minimum of $g(r)$ in order to calculate the six coefficients of the Widom polynomial expressing the screening potential. Their numerical values show some discrepancy compared to MC data and to other works. This point is understandable considering the fact that the extent of the interionic distance examined here is much more important. We intend to improve the correspondence between MC data and our formulation in next papers. The result will can be used to determine the onset of the short range order effect in OCP and then to compare with other works [2, 3].

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