

## LIMITATIONS OF APPLICATION OF YUKAWA POTENTIAL TO FLUID OCP PLASMAS

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### ABSTRACT

After a brief introduction to the Poisson – Boltzmann equation acquired for the one-component-plasmas (OCP), we carry out a careful treatment of the numerical data concerning the radial distribution function given by the Monte Carlo and the Hyper Netted Chain simulations for this kind of plasmas; especially, the weakly correlated ones. Based on some latest results for the screening potential at the near zero inter-nuclear distance, we propose the formulae to compute this potential by combining the Yukawa potential with a certain greater distance than a limit, called Debye-Hückel distance, and the Widom expansion with the lesser one. By this way, we show the limits of application of Yukawa potential to plasmas OCP.

### TÓM TẮT

#### *Giới hạn áp dụng của thế Yukawa cho Plasma OCP lưu chất*

Sau khi giới thiệu ngắn gọn phương trình Poisson – Boltzmann thu được cho plasma một thành phần (OCP), chúng tôi xử lý chi tiết các dữ liệu số liên quan đến hàm phân bố xuyên tâm cho bởi các mô phỏng Monte Carlo và HyperNetted Chain cho loại plasma này, đặc biệt là các plasma liên kết yếu. Dựa trên một vài kết quả mới nhất cho thế màn chắn ở khoảng cách liên hạt nhân gần bằng không, chúng tôi đề nghị các công thức tính thế màn chắn này bằng cách phối hợp thế Yukawa cho khoảng cách lớn hơn một giới hạn gọi là khoảng cách Debye-Hückel, và khai triển Widom cho khoảng cách nhỏ hơn. Bằng cách này, chúng tôi cũng đã chỉ ra những giới hạn áp dụng của thế Yukawa cho plasma OCP.

### 1. Introduction

The Yukawa potential was first introduced into the particle physics to describe the interaction between two nucleons and led to predict the existence of mesons [16]. However, the notion of Yukawa form potential has been widely used in from chemical process to others concerning the astrophysics, and especially considered as a generalization of Debye-Hückel (D-H) potential in the study of the effective potential between two ions separated by the distance  $R$  of a fluid plasma system:

$$V_{\alpha} \propto \frac{e^{-\alpha R}}{R}, \quad (1)$$

wherein  $\alpha$  is a positive parameter characterizing the screening effect of the environment on the two ions under consideration. But the interaction of the form (1)

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above can only be used with some conditions for  $R$  and for the fluidity of the plasmas, as shown in [5, 15]. In this work, by using new computing tools, we will suggest the limits of applying the Yukawa potential (1) for the one component plasmas (OCP) concerning the interionic distance as well as the coupling parameter.

The content of this article will be presented in the following order: Firstly, we remind briefly the model used and the base of D-H theory beginning with the Poisson-Boltzmann equation along with the specifications of applying this theory. Next, we will mention the latest international works related to this subject and indicate at the same time some useful comments for the computations in this work. The following part of this publication will focus on the method used for the treatment of the screening potential in fluid OCP and also on the new results obtained from this study. The conclusion is reserved for the remarks and also for the suggestions.

## 2. Yukawa potential and radial distribution function for fluid OCP plasmas

Within the scope of this work, we consider the model of OCP, that is a physical system at the temperature  $T$ , composed of  $N$  ions, each of  $+Ze$  electrical charge, imbedded in a homogeneous medium of  $ZN$  electrons. This model is suitable for the study of the structure of some astrophysical objects such as the white dwarf or the neutron star,...[9]. An OCP system may be seen as a collection of  $N$  spheres, each centered at one ion and having  $Z$  electrons neutralizing electrical charge. The radius of

this ionic sphere is done by:  $a = \left(\frac{4\pi n}{3}\right)^{-1/3}$ , with  $n$  indicating the ion density. In order

to measure the fluidity of such a OCP system, one uses the coupling parameter, defined

as  $\Gamma = \frac{(Ze)^2}{akT}$ , and dense plasmas the ones which have  $\Gamma > 1$ , meaning that the

Coulomb potential outweighs the thermal energy in magnitude. For some OCP, this parameter has relatively low value, for example, one has  $\Gamma = 0.76$  for brown dwarf and  $\Gamma = 0.072 \div 0.076$  for the solar interior. Especially, in the ICF (Inertial Confinement Fusion) experiments, the magnitude of  $\Gamma$  is only about  $0.002 \div 0.010$ ,... [9]. In these fluid plasmas, the D-H theory is often used to describe the screening effect. The base of this theory will be briefly presented below.

We call  $r = \frac{R}{a}$  the reduced distance and  $y = \frac{V(R)}{Ze/R} \equiv rV(r)$ ,  $V(r)$  being the mean potential at each point of the system, the Poisson-Boltzmann for the OCP system can be described in the compact form [5]:

$$\frac{d^2 y(r)}{dr^2} = 3r \left[ 1 - \exp\left(-\Gamma \frac{y(r)}{r}\right) \right],$$

with the limit conditions:  $\lim_{r \rightarrow 0} y(r) = 1$  and  $\lim_{r \rightarrow \infty} y(r) = 0$ , expressing the interaction potential becomes Coulombian when two ions are near enough so that there no screening effect and it tends to zero when they are too far.

Above some distance, we get this approximative equation:

$$\frac{d^2 y(r)}{dr^2} = 3\Gamma y(r). \quad (2)$$

The solution satisfying those conditions has the expression:

$$y_{DH} = e^{-r\sqrt{3\Gamma}},$$

called Debye-Hückel solution and we have

$$V_{DH} = \frac{e^{-r\sqrt{3\Gamma}}}{r}, \quad (3)$$

a special case of Yukawa potential (1).

At that time, the radial distribution function is described by means of this mean potential:

$$g_{DH}(r) = e^{-V_{DH}/kT} = \exp\left(-\Gamma \frac{e^{-r\sqrt{3\Gamma}}}{r}\right) \quad (4)$$

and if the screening potential is defined as the result of influence of the environment on the interaction between two test ions:  $H(r) = V(r) - \frac{1}{r}$ , we get the following expression for the D-H screening:

$$H_{DH}(r) = \frac{1 - e^{-r\sqrt{3\Gamma}}}{r}. \quad (5)$$

According to (4), the radial distribution function is an strictly increasing function with respect to the distance  $r$ , in accordance with the numerical results of Monte Carlo simulations performed by many authors [1, 8, 13]. On the other hand, those results show that the behavior of this function changes to a kind of damped oscillation from some value of the parameter  $\Gamma_C$ , signature of short-range order effect.

### 3. The conditions of applications of Yukawa potential in fluid OCP plasmas

In order to obtain the equation (2), the condition of linearization must be satisfied, *i.e.* the distance  $r$  must be greater than a certain value  $r_{DH}$  for each  $\Gamma$ . According to [5],

we can use the criterion:  $\varepsilon = \frac{\Gamma y}{2r} \approx \frac{\Gamma e^{-r\sqrt{3\Gamma}}}{2r} < 1$  to evaluate this linearization. On the other hand, for each value of  $\Gamma$ , with  $r \leq r_{DH}$ , the screening potential  $H(r)$  must have

the form of a polynomial whose degree is pair and the coefficient of  $r^2$  is  $h_1 = \frac{1}{4}$ , as demonstrated in [10, 14]:

$$H(r) = h_0 - h_1 r^2 + h_2 r^4 - h_3 r^6 + \dots \quad (6)$$

We see that the functions (5) and (6) must satisfy the continuity condition at point  $r_{DH}$  for each value of  $\Gamma$ , that means:

$$H(r) = \begin{cases} \frac{1 - e^{-r\sqrt{3\Gamma}}}{r} & khi \ r > r_{DH} \\ \sum_{i=0}^{\infty} (-1)^i h_i r^{2i} & khi \ r \leq r_{DH} \end{cases} \quad (7)$$

#### 4. Determine the Widom polynomial coefficients

The data concerning the coefficient  $h_0$  of the polynomial (6) have been the subject of many discussions for its important role in the enhancement of the pycnonuclear reaction rate in some stellar objects with great mass density as white dwarfs, neutron stars, ... (See, for example, [3, 9, 12]). The latest MC simulations implemented by A. I. Chugunov *et al* [2] supply the value of  $h_0$  in a analytic form:

$$h_{0CHU} = \Gamma^{1/2} \left( \frac{A_1}{\sqrt{A_2 + \Gamma}} + \frac{A_3}{1 + \Gamma} \right) + \frac{B_1 \Gamma}{B_2 + \Gamma} + \frac{B_3 \Gamma}{B_4 + \Gamma^2} \quad (8)$$

with:

$$A_1 = 2,7822, \quad A_2 = 98,34, \quad A_3 = \sqrt{3} - A_1 / \sqrt{A_2} = 1,4515,$$

$$B_1 = -1,7476, \quad B_2 = 66,07, \quad B_3 = 1,12, \quad \text{và} \quad B_4 = 65.$$

One of the characteristics of this expression is one can obtain the asymptotic form  $h_{0CHU} = \sqrt{3}\Gamma^{1/2}$  with small values of  $\Gamma$ . We recognize that the value of  $h_0$  of those two expressions coincide (with errors 0.3%) from  $\Gamma \leq 0.0032$ , *i.e.* for very fluid plasma.

In opposition to the MC simulations that give us the relatively exact of the radial distribution function for the dense plasmas, the HyperNetted Chain (HNC) calculations are more reliable for the fluid OCP systems [11]. An elaborate study of the MC and HNC data [1, 4, 13] show that for not too important magnitude of the coupling parameter:  $\Gamma \leq 10$ , we can write the Widom polynomial of degree eight with the error about 0.2%, equivalent to that of MC simulations, that means we accept:

$$H(r) = h_0 - \frac{1}{4} r^2 + h_2 r^4 - h_3 r^6 + h_4 r^8 = \sum_{i=0}^4 (-1)^i h_i r^{2i}. \quad (9)$$

as the expression for the screening potential for enough small interionic distances.

By optimizing the accordance between the polynomial (9) and the MC as well as the HNC data given by [1, 4, 13], one gets all the numerical values of the coefficients  $h_i$  in (9). Especially, the numerical value of  $h_0$ , presented in Table 1, can be expressed in a analytic form:

$$h_0 = \frac{\sqrt{3\Gamma}}{1+\Gamma} + \sum_{i=1}^5 a_i \ln^i(1+\Gamma) \quad (10)$$

with the coefficients  $a_i$  given by:

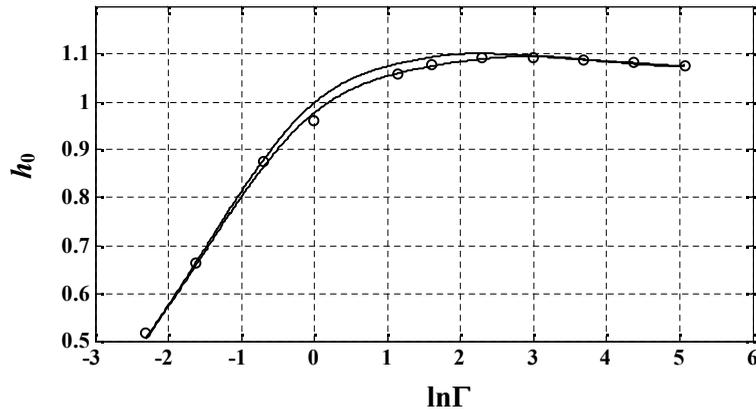
$$a_1 = 0,031980; a_2 = 0,232300; a_3 = -0,084350;$$

$$a_4 = 0,011710; a_5 = -0,000579.$$

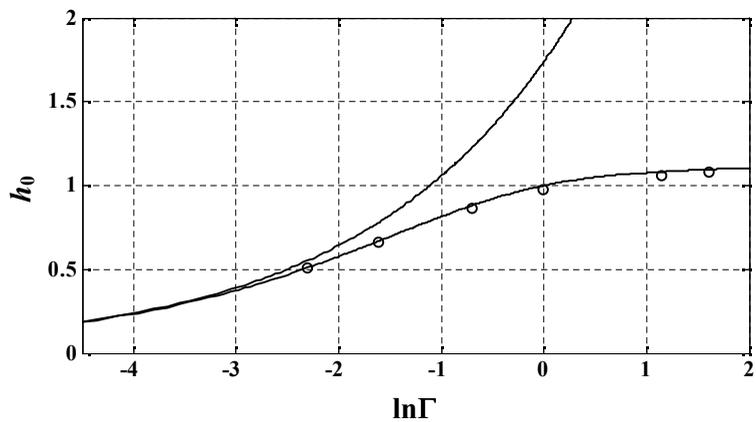
The error between (8) and (10) is shown in Table 1. We notice that those both expressions give:  $\lim_{\Gamma \rightarrow 0} h_0 = \sqrt{3\Gamma}$  as we can see on the Figure 2.

**Table 1. Numerical values of  $h_0$  in function of  $\Gamma$ .** *The values of  $h_0$  directly obtained from the optimization the accordance between (6) and MC and HNC data, and computed from (9) are shown in the second and third columns. In the fourth column, we have the values of  $h_0$  according to Chugunov et al [2].*

$\Gamma$	$h_{0MC}$ (2)	$h_0$ (3)	$h_{0CHU}$ (4)	(3) - (2)	(4) - (2)	(3) - (4)
<b>0,1</b>	0,5150	0,5030	0,5050	-0,0120	-0,0100	-0,0020
<b>0,2</b>	0,6615	0,6589	0,6645	-0,0029	0,0030	-0,0059
<b>0,5</b>	0,8741	0,8623	0,8776	-0,0118	0,0035	-0,0152
<b>1</b>	0,9586	0,9743	0,9958	0,0157	0,0372	-0,0215
<b>3,1748</b>	1,0570	1,0586	1,0788	0,0016	0,0218	-0,0201
<b>5</b>	1,0780	1,0735	1,0922	-0,0045	0,0142	-0,0187
<b>10</b>	1,0920	1,0888	1,1007	-0,0032	0,0087	-0,0119
<b>20</b>	1,0910	1,0940	1,0950	0,0030	0,0040	-0,0010
<b>40</b>	1,0860	1,0882	1,0878	0,0022	0,0018	0,0004
<b>80</b>	1,0810	1,0782	1,0804	-0,0028	-0,0006	-0,0022
<b>160</b>	1,0750	1,0757	1,0737	0,0007	-0,0013	0,0020



**Figure 1.** The solid line expresses the formula (10) compared with the dashed line for (8). The circles are values directly acquired from optimizing the agreement between (7) and MC and HNC data.



**Figure 2.** The solid line expresses (10). The circles are MC and HNC values given in Table 1. The dashed line is the asymptotic behavior  $\sqrt{3\Gamma}$ .

We can notice that another expression for  $h_0$  is also proposed for dense plasmas in [6]. However, the formula (10) satisfies the particular conditions for the fluid plasmas we shall need for the use of the Yukawa potential for this category of plasmas.

The method mentioned above give us at the same time the numerical values for the other coefficients  $h_2, h_3,$  and  $h_4$  as seen in Table 2.

**Table 2.** Numerical values of the coefficients in the Widom polynomial (9).

$\Gamma$	$h_2$	$h_3$	$h_4$
<b>0,1</b>	0,285915	0,155198	0,0298883
<b>0,2</b>	0,184492	0,077716	0,0122415
<b>0,5</b>	0,074081	0,0127690	0,00088438
<b>1</b>	0,051772	0,0062949	0,00033008
<b>2</b>	0,040241	0,0032605	0,00009693
<b>3,174802</b>	0,035570	0,0020166	0,00000154

All the numerical values of these coefficients can be found by the general analytic expression:

$$h_i = \sum_{k=0}^5 b_k (\ln \Gamma)^k ; i = 2, 3, 4 \quad (11)$$

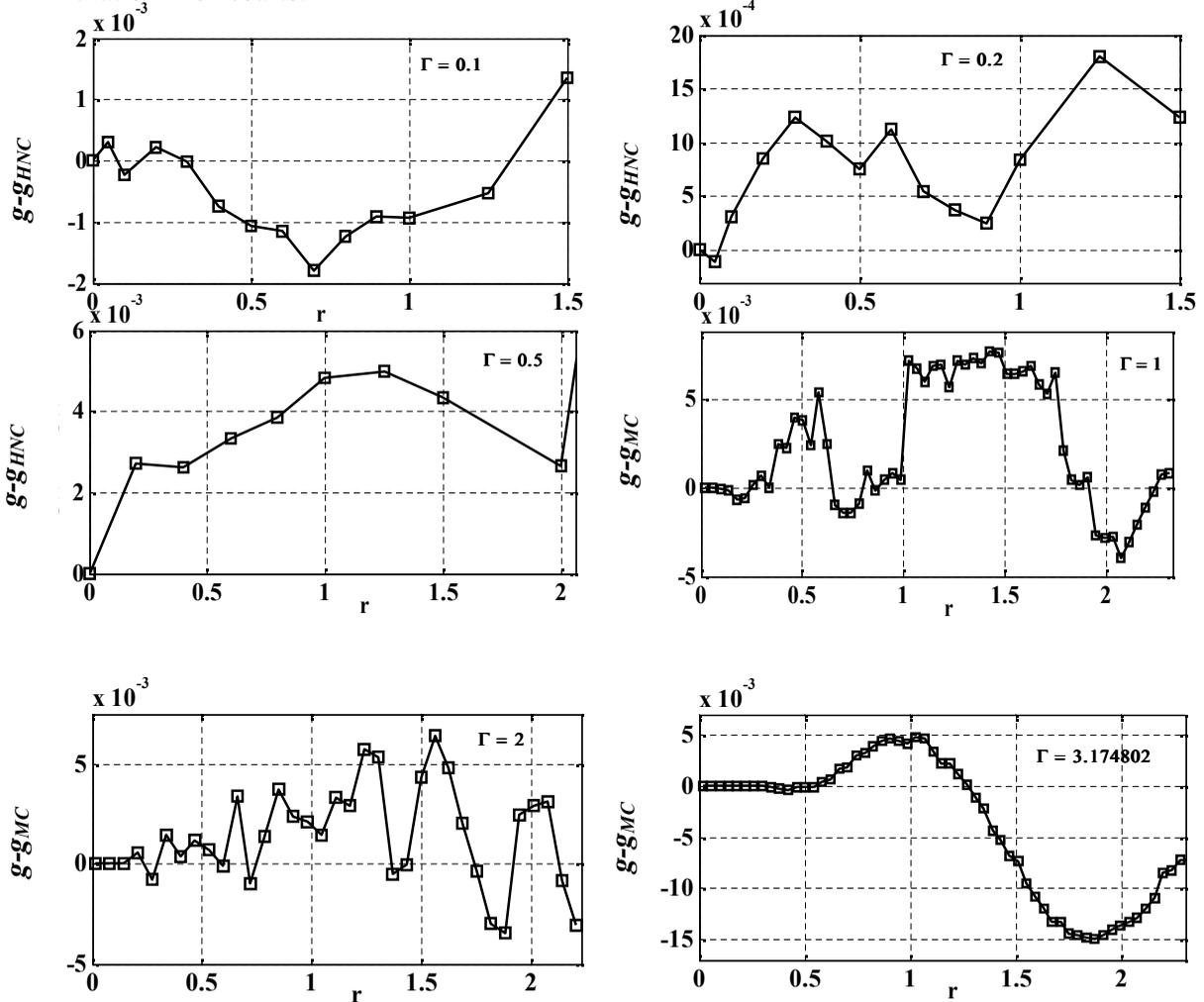
with values of  $b_k$  shown in Table 3. A study of the variation of  $h_i$  in function of  $\Gamma$  demonstrates that their behavior is uniformly decreasing without any unusual point.

**Table 3.** The coefficients in the formula (11) computing  $h_i$ .

	$h_2$	$h_3$	$h_4$
$b_0$	0,05177	0,006295	0,0003301
$b_1$	-0,01518	-0,0004388	0,0005552
$b_2$	0,007324	0,0004114	-0,0002833
$b_3$	-0,02167	-0,01502	-0,002602
$b_4$	0,008098	0,006594	0,001285
$b_5$	0,005127	0,003445	0,0005493

With the numerical values obtained from the formulae (10) and (11), we can compute the function of screening potential (9) and from that point, return to evaluate the radial distribution function  $g(r)$ . The comparison of this with the MC and HNC results is given on Figure 3 for some values of  $\Gamma$ . The data concerning  $\Gamma = 2$  are quoted from [8]. We notice on the Figure 3 that the errors between the proposed

analytical formulae and the simulation data are about some thousandths, equivalent to that of MC results.



**Figure 3.** Errors  $g(r) - g_{MC}(r)$  or  $g(r) - g_{HNC}(r)$  between the radial distribution function  $g(r)$  deduced from (10) and (11) and MC or HNC data for each value of  $\Gamma$ .

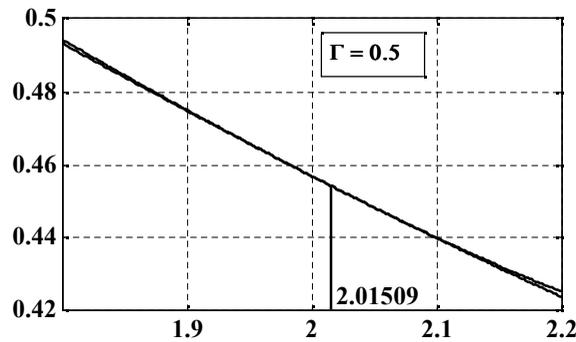
### 5. Limit $r_{DH}$ for each value of coupling parameter

When one accepts that the D-H potential can only be used from interionic distance  $r_{DH}$  for each  $\Gamma$ , the continuity conditions (7) will be applied for the amplitude of the functions:

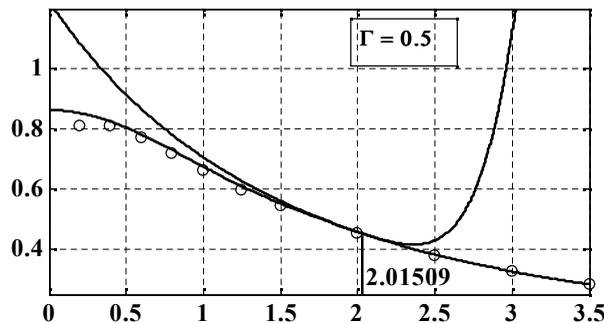
$$H(r)|_{r=r_{DH}} = \frac{1 - e^{-r_{DH}\sqrt{3\Gamma}}}{r_{DH}} = h_4 r_{DH}^8 - h_3 r_{DH}^6 + h_2 r_{DH}^4 - h_1 r_{DH}^2 + h_0 \quad (12)$$

to find those values  $r_{DH}$ . An example is given on the Figure 4a and 4b for  $\Gamma = 0,5$ : We see that only from points with  $r > r_{DH} = 2,01509$ , an expression of the form (5) can be consistent to the numerical data offered by HNC method. This remark shows that for the distance smaller than  $r_{DH} = 2,01509$ , D-H potential is not suitable to describe the screening effect

The common results of  $r_{DH}$  for each value of  $\Gamma$  are presented on Table 4, which show more clearly the limit of application of D-H theory.



**Figure 4b.** At the point whose abscissa is 2,01509, two line representing  $H(r)$  and  $H_{DH}(r)$  intersect and have almost the same slope.



**Figure 4a.** From the points whose abscissa is smaller than 2,01509, the D-H potential (dash line) must be replaced by the Widom expansion (solid line). The circles are HNC data.

**Table 4. The numerical value of the joint points between the D-H potential and Widom polynomial.**

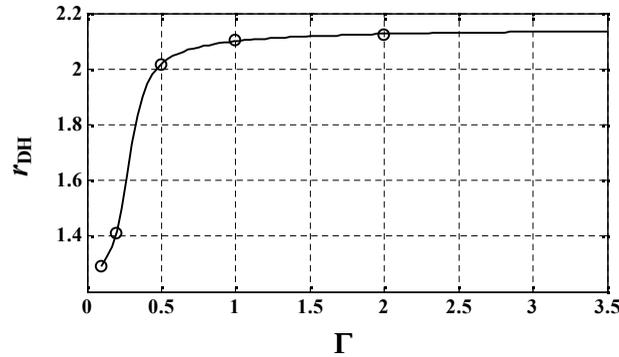
$\Gamma$	$r_{DH}$
0,1	1,29072
0,2	1,40899
0,5	2,01509
1	2,09863
2	2,12295

The numerical values on Table 4 can be expressed by analytic function:

$$r_{DH} = 1,69 + 0,3059 \arctan(3,394 \ln \Gamma + 4,156). \quad (13)$$

In order to see more [ further] the importance of the Widom polynomial in representing the screening potential, we can observe on the Figure 5 the variation of  $r_{DH}$  with respect to  $\Gamma$  according to (13): The value of  $r_{DH}$  increasing in function of  $\Gamma$  shows that the Yukawa potential expresses accurately the screening effect only for fluid plasmas and, and even then, this form of potential can be applied only with large enough distances  $r$ .

The expression (13) presented above has a simpler form, more easily applied than the one proposed in [5], while the maximum error between them is only about 9% for  $\Gamma = 0,1$ .



**Figure 5.** The variation of  $r_{DH}$  with respect to  $\Gamma$ . We see that the influence of the Yukawa potential decreases when the plasmas are denser.

It is interesting to notice that apart from the condition (12) expressing the continuity of the amplitude, one should verify the continuity of the slope of the two functions (5) and (9) as well as insure they have the same concavity at the joint point  $r_{DH}$ , i.e.:

$$\left\{ \begin{aligned} \frac{\partial}{\partial r} H(r)|_{r=r_{DH}} &= \frac{\sqrt{3\Gamma} e^{-r_{DH}\sqrt{3\Gamma}}}{r_{DH}} + \frac{e^{-r_{DH}\sqrt{3\Gamma}} - 1}{r_{DH}^2} = 8h_4 r_{DH}^7 - 6h_3 r_{DH}^5 + 4h_2 r_{DH}^3 - 2h_1 r_{DH} \\ \frac{\partial^2}{\partial r^2} H(r)|_{r=r_{DH}} &= -\frac{2(e^{-r_{DH}\sqrt{3\Gamma}} - 1)}{r_{DH}^3} - \frac{2\sqrt{3\Gamma} e^{-r_{DH}\sqrt{3\Gamma}}}{r_{DH}^2} - \frac{3\Gamma e^{-r_{DH}\sqrt{3\Gamma}}}{r_{DH}} = 56h_4 r_{DH}^6 - 30h_3 r_{DH}^4 + 12h_2 r_{DH}^2 - 2h_1 \end{aligned} \right.$$

The more concrete calculations show that the first and second derivatives for each value of  $\Gamma$  of the two functions (5) and (9) at the point  $r = r_{DH}$  have the same values with very small errors (the maximum error is about  $10^{-11}$ ). This affirms the accuracy of the numerical values of  $r_{DH}$  on the Table 4 and of the expression (13).

## 6. Conclusion

We consider in detail the D-H potential, a special case of Yukawa potential, applied to the fluid OCP system and mention the conditions for the application of this theory.

After an elaborate study of the MC and HNC data as well as of the newest publications, we perform the numerical calculations and suggest the formula (13) for the limit distance of application of the D-H potential indicating that for each value of the parameter  $\Gamma$ , at the interionic distances smaller than this limit, this form of potential should be replaced by a Widom polynomial of degree eight (9) with the coefficients also expressed by the analytic formulae (10) and (11). The results obtained from the proposed expressions have also been compared with the numerical data for the distribution function  $g(r)$ ; the discrepancy between those two values is conform to the expected exactitude.

In the following works, we will especially consider the short-range order effect in the various plasmas, that is the onset of damped oscillations of the distribution function, and then, to study the apparition of this effect in function of the coupling parameter  $\Gamma$ . At the same time, we will focus on the determination of the value of  $\Gamma$  for which the Yukawa potential can accurately express the screening potential in plasmas.

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