SCREENING POTENTIAL AT THE CRYSTALLIZATION POINT OF ULTRADENSE OCP PLASMAS

DO XUAN HOI*, PHAN CONG THANH**

ABSTRACT

With a very elaborate method, we verify the accuracy of the screening potential (SP) computed by the consideration of the short range order effect for the classical One-Component-Plasmas (OCP). We obtain a compact, effective form for the SP, useful for the computerization and find the exact value of Jancovici coefficient. The agreement between our formula and the Monte Carlo simulation data proves completely satisfactory. As a result, the calculation for this quantity can be extended by an extrapolation to the region where the crystallization of the OCP system is thought to appear and the expression for the SP at this phase change point will be presented.

Keywords: OCP system, screening potential, pair correlation function, Monte Carlo simulations, extrapolation, crystallization point, analytical formula.

TÓM TẮT

Thế màn chắn tại điểm kết tinh của plasma siêu đậm đặc

Chúng tôi sử dụng một phương pháp rất tinh vi để kiểm chứng lại tính chính xác của thế màn chắn (TMC) của hệ Plasma Một thành phần (OCP) cổ điển đã được tính toán dựa trên việc nghiên cứu hiệu ứng trật tự địa phương. Chúng tôi có được một dạng cô đọng, có hiệu quả cho TMC, hữu ích cho việc tính toán trên máy tính và tìm được giá trị chính xác của hệ số Jancovici. Sự tương hợp giữa các công thức của chúng tôi đề nghị và dữ liệu mô phỏng Monte Carlo là hoàn toàn thỏa đáng. Kết quả trên cho phép chúng tôi mở rộng phép tính TMC bằng phương pháp ngoại suy đến vùng kết tinh của hệ OCP và trình bày biểu thức của TMC tại điểm chuyển pha này.

Từ khóa: Plasma OCP, thế màn chắn, hàm tương quan cặp, mô phỏng Monte Carlo, phép ngoại suy, điểm kết tinh, công thức giải tích.

1. Introduction

As pointed out in several works related to the study of ultradense plasmas, the crystallization occurs when the ratio of the Coulomb potential and the thermal one reaches a certain value; the order structure takes form and a bcc lattice is thought to appear in classical one component plasmas (OCP). In this simplest model of OCP, the relation between the Coulomb interaction and the random motion of the ions of charge Ze in a plasma system is characterized by the correlation parameter: $\Gamma = \frac{(Ze)^2}{akT}$ where kT is thermal kinetic energy and a is ion sphere radius. The fluid – Wigner solid phase transition is of great importance in the study of some stellar objects of high density such as the cooling White Dwarfs and the accreting neutron stars [9, 10].

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In this work, we develop a method allowing to obtain highly accurate screening potential (SP) for various value of the parameter Γ for the fluid OCP, so that a study of OCP can be extended from the liquid phase to the its crystalline state. Up till now, there have been numerous simulations giving the value of pair distribution function $g(r)$ and the internal energy $u(\Gamma)$ of an OCP system. The function $g(r)$ is related to the potential of mean force $V(R = ar)$ through $g(R) = \exp\left[-\beta V(R)\right]$, where $\beta = \frac{1}{kT}$ is inverse of characteristic energy. The SP is then defined by: $H(R) = \frac{(Ze)^2}{R} - V(R)$, which characterizes the influence of the medium on the electric interaction between two ions. In one of previous works [13], we have proposed a method based on the parametrization of the short range order effect in an OCP system, which allows to reproduce the value of the pair distribution function $g(r)$. In this work, we shall continue to use the MC simulations results proposed by DeWitt *et al* [4], which, up to this day, is still considered to be the most exact one concerning the data of $g(r)$. As a matter of fact, some of the thermodynamic functions of this OCP system at the phase transition point will be clarified.

The determination of the value of the SP $H(r)$ for a certain value of the parameter Γ and for some value of the interionic distance r is based on those two characteristics of $H(r)$: First of all, this function must be expressed in form of an even degree polynomial alternate in sign in powers of r [14]:

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

And then, the second criterion for an exact form of $H(r)$ is that the value of the coefficient h_1 in (1) has been demonstrated to be $\frac{1}{4}$ [8]. Using the method of least square, we verify the correspondence of this calculation to the parametrization of the short range order effect [13]. Anyway, if in [13], the value $\frac{1}{4}$ is *accepted* for the coefficient h_1, we will point out that this value can be obtained naturally without any constraint.

2. Implementation of calculation and results of least square method for $1 \leq \Gamma \leq 160$

We have carried out the computation of the SP $H(r)$ for the extent of the distance from r ; 0 to r ; 2.7 and for the wide range $1 \leq \Gamma \leq 160$, including in this way the plasmas fluid and dense, accepted the polynomial of twelfth degree:

$$H(r) = h_0 - h_1 r^2 + h_2 r^4 - h_3 r^6 + h_4 r^8 - h_5 r^{10} + h_6 r^{12} . \quad (2)$$

The flowchart of the computation using the least square method is shown in Figure 1 [3].

One can notice that the criteria for the form of the polynomial (2) as well as the Jancovici coefficient are strictly obeyed.

The result for the coefficients of the SP (2) is given in the Table 1 [3]. And in Table 2, we show the difference between two series of numerical values for h_i with $\Delta h_i = h_i - h_{iDXH}$ of which h_i is the value obtained in this work and h_{iDXH} is the one found in [2, 13]. This presents a surprising agreement between the two series of values, once again proves the effectiveness of the method of parametrization of the short range order effect.

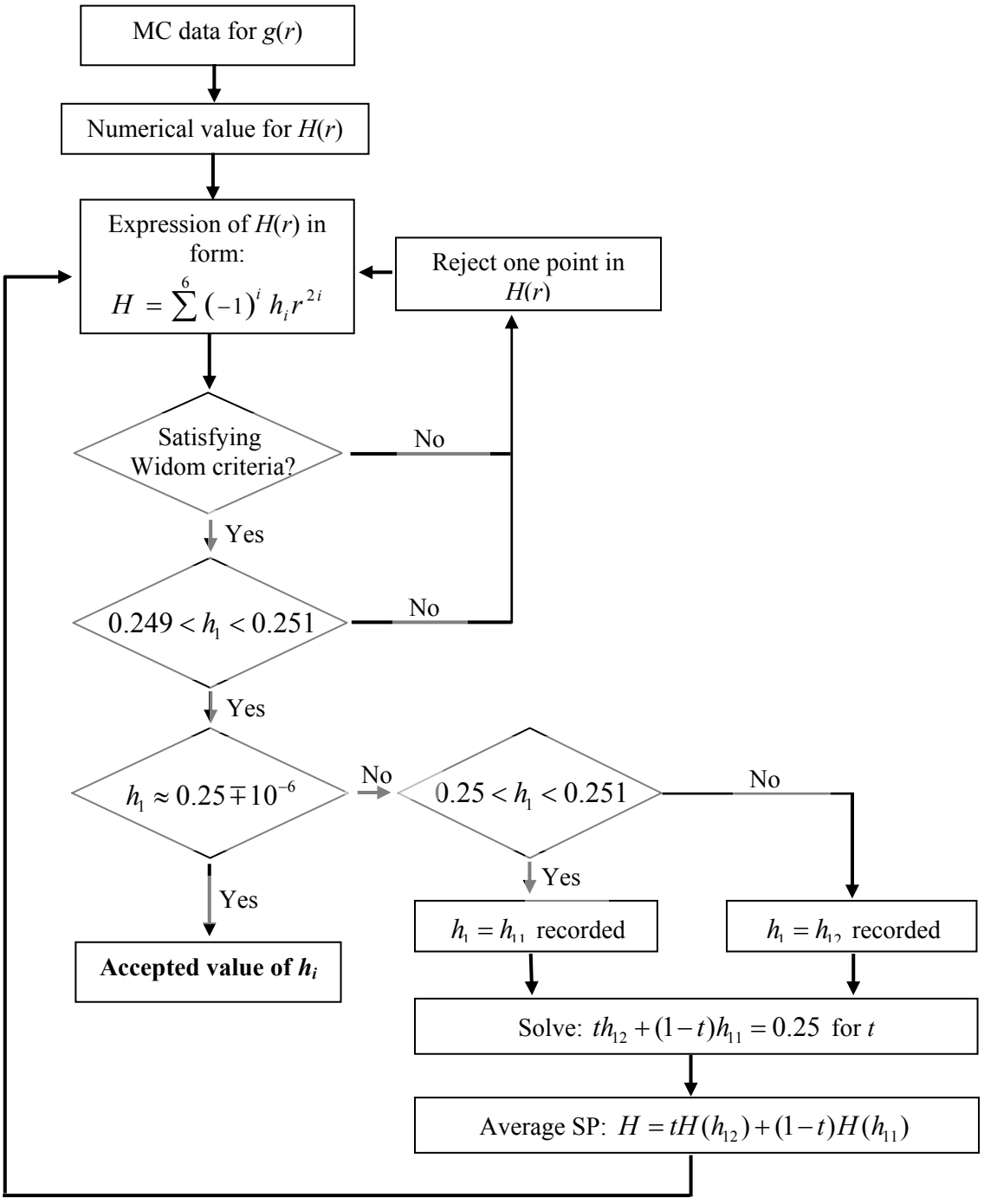

Figure 1. *Process of the fitting for H(r)*

Table 1. *Numerical value for* h_i

Γ	h_0	$10h_1$	10^2h_2	10^3h_3	10^4h_4	10^5h_5	10^6h_6
1	0.9398	2.49999997	6.72814397	14.07334218	19.76818196	15.81103621	5.32444504
3.17	1.052720435	2.50000000	3.95512311	3.29365929	1.11452982		
5	1.074451980	2.50000000	3.59005255	2.52542680	0.88548351	0.62615106	0.44785592
10	1.087820610	2.50000005	3.54326653	3.20047994	3.34030120	3.54755254	1.65016650
20	1.089190262	2.500007	3.51967025	3.02450713	2.50013212	2.05173727	0.79097283
40	1.085364578	2.500000000	3.51480100	2.75290800	1.57651000	0.91200000	0.30600000
80	1.079751445	2.50000000	3.55162522	2.73277476	1.42661077	0.82185439	0.32068040
160	1.074578527	2.50000011	3.57402220	2.63111500	1.08302000	0.50413717	0.22851037

Table 2. *Comparison of numerical values for* h_i *in this work and in* [2, 13]

Γ	Δh_0	$10\Delta h_1$	$10^2\Delta h_2$	$10^3\Delta h_3$	$10^4\Delta h_4$	$10^5\Delta h_5$	$10^6\Delta h_6$
5	0.009462	0	1.387288	4.548847	7.438716	5.847449	1.737244
10	0.008419	0	1.282038	4.743555	-3.21554	8.776447	3.315434
20	0.007052	0	0.686789	2.017584	3.076068	2.331263	0.691327
40	0.004745	0	0.40806	1.171316	1.78909	1.3914	0.4338
80	0.003075	0	0.173338	0.365945	0.341989	0.079546	-0.03998
160	0.002496	0	0.091984	0.106902	-0.08412	-0.27344	-0.15741

The first remark is whether in [2, 13], the coefficients h_i can be computed only for high density plasmas with $\Gamma \geq 5$ and for fluid plasma, another technique is required [5], here, we present all the values for both these categories of plasmas. Based on this accuracy, we think we can extend the field of interest into larger value of the correlation parameter. The second notice worth being underlined is that in the third columns of the tables, the Jancovici value for h_1 is demonstrated to be $\frac{1}{4}$ by computing for the first time with very accurate value of the pair correlation function $g(r)$ comparing with the MC data. In comparison with one of our previous works as far as the first coefficient h_0 is concerned [1], we can recognize some discrepancy. This will reflect in the evaluation of the pycnonuclear reaction rate as many authors have pointed out [12].

3. Extrapolation for ultradense plasmas and the general result. The SP at the crystallization point

With the intention to study the value of the SP at the critical value of correlation parameter Γ where exists the phase change from fluid state to the bcc crystal, we extend our work to the plasmas with $\Gamma \geq 160$. Notice that we do not benefit any MC simulation data of the pair correlation function for this range of Γ. As a matter of fact, we put forward here an extrapolation method to obtain these data. Instead of fitting the SP for each value of Γ, we choose another approach: By considering the value of the SP for various value of the distance *r* for each one value of Γ, we recognize that for Γ > 40, the range of this parameter that we focus on, the SP has a almost linear variation with respect to lnΓ for a quite wide range of *r*, as we can see in Figure 2. With this surprising remark, and accepting that the SP must take continuous value when Γ varies, we can proceed and acquire this way the SP for all the missing values of Γ. We present some of those values which are interesting for this work in the Table 3. A comparison with the SP obtained by the least square method for $1 \leq \Gamma \leq 160$ is also made and the consistency is perfect. Moreover, the Jancovici coefficient of the Widom polynomial (2) has the almost exact value $\frac{1}{4}$. This point may give us some idea about the exactness of the method applied here.

Table 3. *Numerical values of the SP for the extremely dense OCP*

Γ	h_0	$10h_1$	10^2h_2	10^3h_3	10^4h_4	10^5h_5	10^6h_6
100	1.07798329	2.5000000	3.56532849	2.74398644	1.43467678	0.86091546	0.35229755
110	1.07725378	2.5000000	3.57004535	2.74160689	1.41908713	0.85455329	0.35544999
120	1.07660400	2.5000000	3.57336478	2.73278035	1.38686121	0.82726088	0.34898617
130	1.07602100	2.4999999	3.57534682	2.71725297	1.33709341	0.77828476	0.33279433
140	1.07549441	2.4999999	3.57606486	2.69502149	1.26962633	0.70769337	0.30706470
150	1.07501586	2.4999999	3.57559699	2.66623086	1.18474873	0.61603060	0.27215286
155	1.07479242	2.4999999	3.57494280	2.64944567	1.13594605	0.56254416	0.25138938
165	1.07437351	2.4999999	3.57284156	2.61126350	1.02603165	0.44084021	0.20354274
172	1.07410026	2.4999999	3.57077368	2.58100468	0.93965163	0.34439386	0.16524852
175	1.07398774	2.4999999	3.56974399	2.56717648	0.90032959	0.30032425	0.14767485
175.3	1.07397663	2.4999999	3.56963641	2.56576578	0.89632274	0.29582874	0.14587996
178	1.07387637	2.5000000	3.56858336	2.55240432	0.85849542	0.25344891	0.12900374
178.6	1.07385613	2.4999998	3.56839844	2.54991788	0.85136284	0.24532945	0.12569224

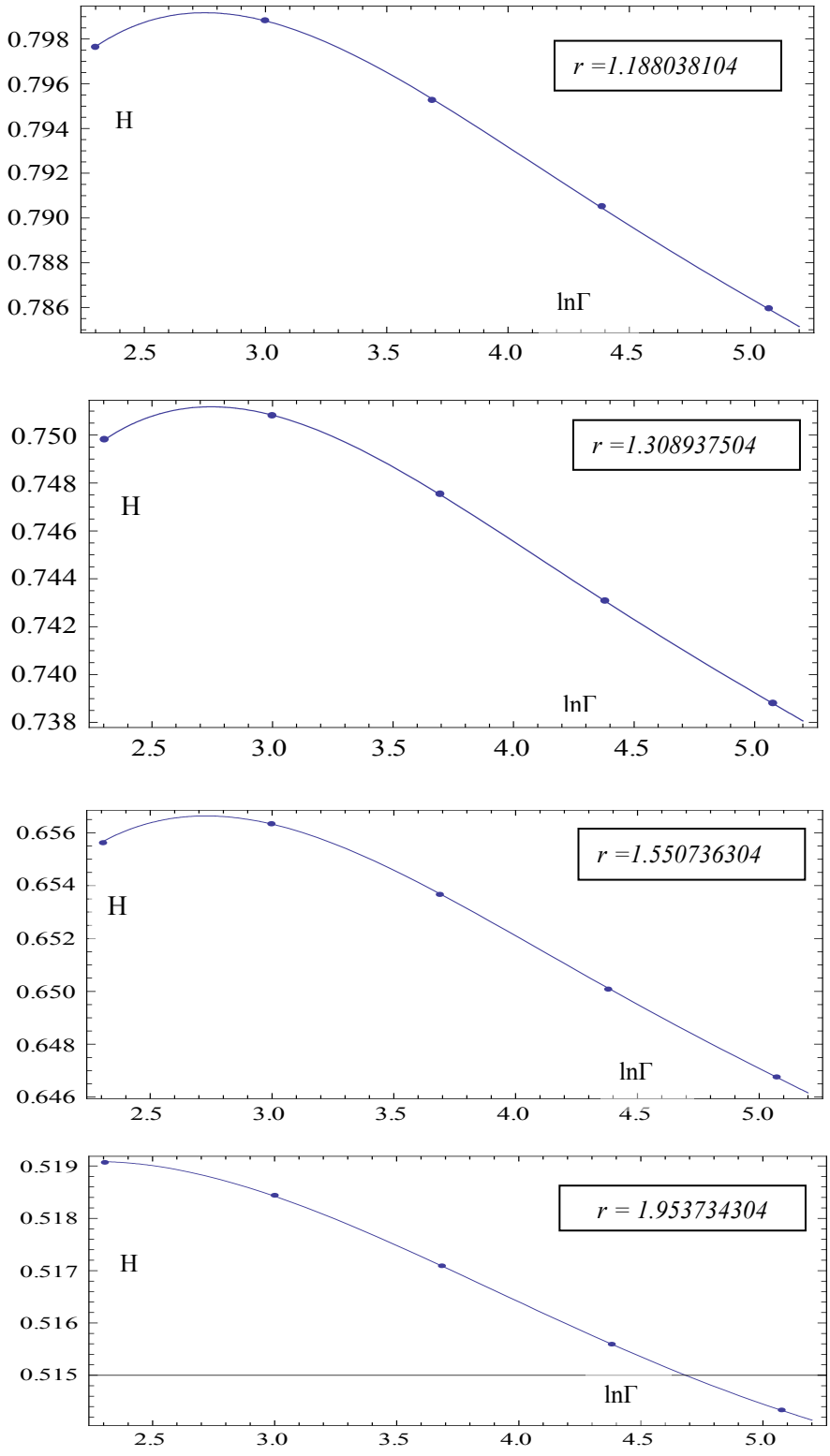

Figure 2. *The remarkable behavior of the SP with Γ varied for a fixed value of r*

In order to give some ideas of this good agreement, we show the variation of the absolute error between the value of $g(r)$ in this work and that of MC simulation in Figure 3. As we can see, the discrepancy is very small, about 0.2×10^{-3} for Γ = 10, 20 and 80. Furthermore, the extent of the ionic distance is until r = 2.8 for some values of Γ.

To provide a useful formula to the numerical value of the SP for any correlation parameter, which can be easy to adapt to computing programs, we propose:

$$H\left(r\right)=\sum_{i=0}^{6}(-1)^{i}h_{i}r^{2i} \tag{3}$$

$$h_{i}=10^{-i}\sum_{k=0}^{4}a_{k}^{i}\left(\ln\Gamma\right)^{k} \tag{4}$$

where the coefficients a_k^i are taken from the Table 4 [11].

Table 4. *Numerical value for the coefficient a_i in (4)*

	h_0	h_2	h_3	h_4	h_5	h_6
a_0	0.97105763	1.86641885E-2	-1.50481749E-2	4.22041597E-2	-3.75237952E-4	-9.1740129E-6
a_1	0.11507638	2.18979861E-2	2.22553292E-2	5.72361242E-2	5.54314838E-4	1.7065102E-5
a_2	0.03875562	1.02577323E-2	9.75701536E-3	2.56608866E-2	2.62047147E-4	8.8858804E-6
a_3	0.00529728	2.02742303E-3	1.81759492E-3	4.83882060E-4	5.10972174 E-5	1.8315623E-6
a_4	2.633932E-4	1.43009964E-4	1.22929974E-4	3.29772061E-5	3.56158477E-6	1.3227440E-6

We can notice that, considering the small magnitude of the fifth and sixth coefficients in the Table 4, instead of a twelfth degree polynomial for the SP proposed in our previous works [2, 13], the appropriate form for the Widom expression should be a eighth degree polynomial. This point must be very useful in computer calculations of the field of interest.

Provided with the general expressions (3), (4), and the Table 4, we now can explore the SP at the crystallization point. According to [7], at the value Γ = 172, there exists a coexistence between a Wigner bcc crystal and a fluid plasma, some SP expressions for this value of the correlation parameter have been proposed, for example, in [6]:

$$H_{DXH}(r)=1.0521-0.25r^{2}+0.04392r^{4}-0.004269r^{6}\qquad r\in[0.0,2.0] \tag{5}$$

Or in [11]:

$$H_{OII}(r)=\begin{cases}1.0605-0.25r^{2} & r\in\left[0.0,0.7\right]\\ 1.10830-0.35r+\dfrac{1}{r}\exp\left(13.2\sqrt{r}-22.1\right) & r\in\left[0.7,2.0\right]\end{cases} \tag{6}$$

We propose here another formula:

$$H(r) = 1.074100 - 0.25r^2 + 3.570774.10^{-2}r^4 - 2.581005.10^{-3}r^6 + 0.939652.10^{-4}r^8 \\ 0.344394\times10^{-5}r^{10} + 0.165248\times10^{-6}r^{12} \quad (7)$$

In Figure 4, we notice the agreement between (5) and (6), the latter comes from MC data carried out some time before those used in this work. It is also pronounced in this figure the discrepancy between the three formulae concerning the SP near the phase change fluid-solid: While the SP in (5) and (6) represents a relative sharp decrease and tends to take negative value for the interionic distance $r \geq 2.6$, the expression (7) seems to have more reasonable behavior for a quite large range of *r*. Anyway, one feature which is worth remarking concerns the SP value at the distance r ; 0, where there happens the nuclear reaction and the magnitude of

H(*r* = 0) plays an important role in the evaluation of the reaction rate [1]. This point will be considered in another work.

Moreover, according to the last updated works, the crystallization of an OCP system occurs for a slightly larger value of the correlation parameter. For example, in [10], the free energy difference between the solid and liquid phase is studied carefully and a phase transition between the liquid and solid state for $\Gamma = 175.3$. Or in [9], the authors perform molecular dynamics simulations for a pure 27648 carbon ions and observe that the melting value of Γ is 178.4 ± 0.2. We put forward here the two expressions of the SP for $\Gamma = 175$ and $\Gamma = 178$ respectively:

$$H_{175}(r) = 1.073988 - 0.25r^2 + 3.569744\times10^{-2}r^4 - 2.567177\times10^{-3}r^6 + 0.900330\times10^{-4}r^8 \\ - 0.300324\times10^{-5}r^{10} + 0.147675\times10^{-6}r^{12} \quad (8)$$

And

$$H_{178}(r) = 1.073876 - 0.25r^2 + 3.568583\times10^{-2}r^4 - 2.552404\times10^{-3}r^6 + 0.858495\times10^{-4}r^8 \\ - 0.253449\times10^{-5}r^{10} + 0.129004\times10^{-6}r^{12} \quad (9)$$

Those two formulas (8) and (9) will be of high interest when we consider the value of the pair correlation function *g*(*r*) for $\Gamma = 175$ and $\Gamma = 178$. In fact, we can observe a continuity of *g*(*r*) with a series of $\Gamma = 40$, $\Gamma = 80$, $\Gamma = 160$ (supplied by MC simulations), to $\Gamma = 175$ and $\Gamma = 178$. This is also another proof of the consistency in the model of our calculation.

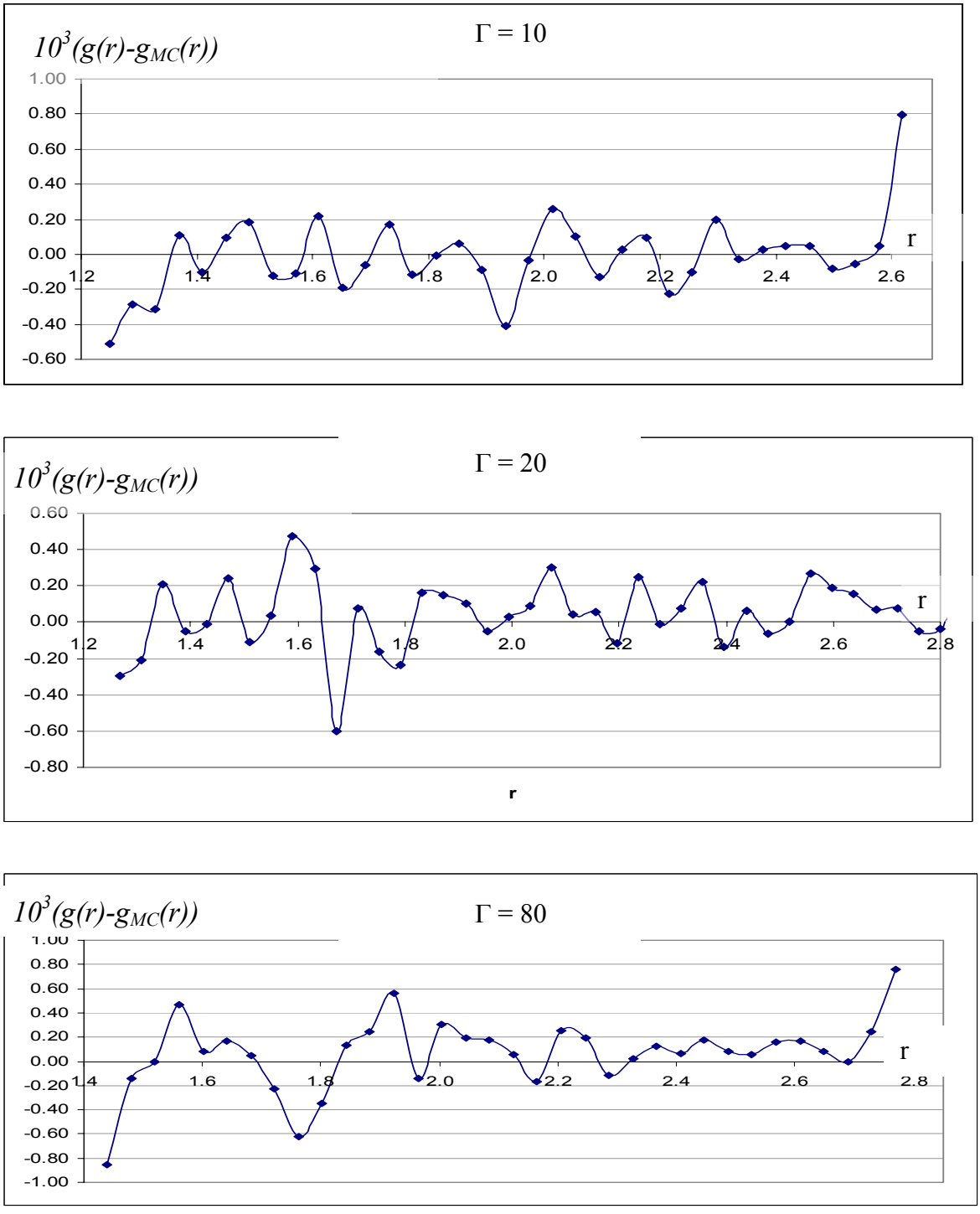

Figure 3. *Comparison of fitted and MC values for various values of Γ*

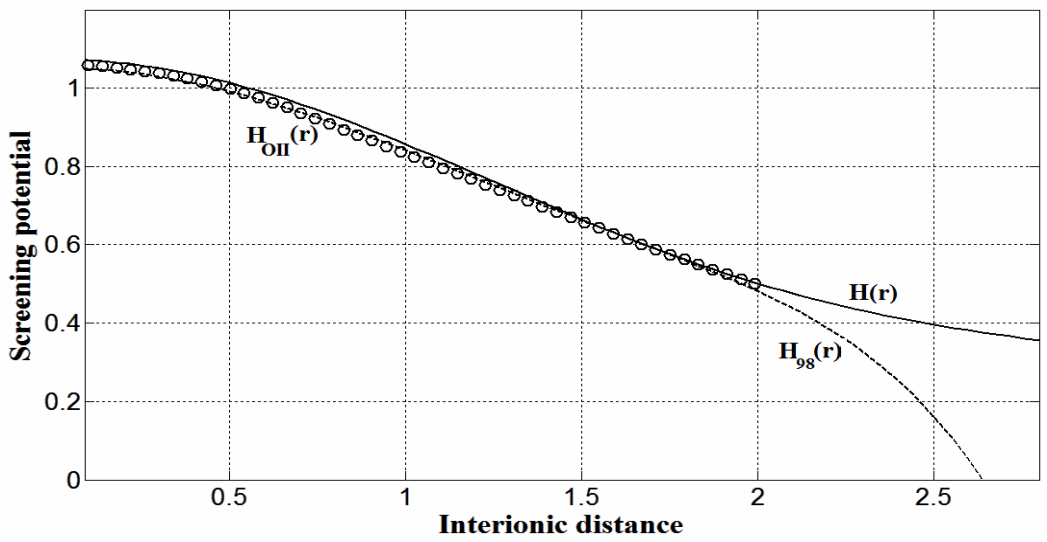

Figure 4. *Variation of the SP with respect to the interionic distance. Solid line: H(r) in this work, Broken line: The SP in [6], Dotted line: The SP in [11]*

4. Conclusion

In this work, we have developed a method which gives us an extremely accurate result for the SP of a classical OCP system, from dilute fluid to ultradense state. We obtain this way a more concise expression (3) for the SP: a polynomial of twelfth degree giving the same accuracy as the form presented in other work. Moreover, in our computation, the Jancovici coefficient appears in a very natural way and it is the first time this coefficient is found with such exactness. Based on an extrapolation from these numerical values, we can also deduce the SP for the crucial value of the correlation parameter where there exists the fluid- solid phase change. The result of this work will introduce an important impact on the parametrization of the SP and also on the evaluation of the nuclear reaction rate which occurs in some very dense stellar objects.

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