Screening potential in lattices and high-density plasmas

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(Received 16 July 1997; revised manuscript received 18 November 1997)

The screening potential in a body-centered-cubic (bcc) crystal has been calculated in detail and expressed as a series expansion including the hexadecapole term for small displacements from the equilibrium configuration and also as a closed-form fitting numerical lattice sums performed for the larger ones. We have shown that this closed form is an even function of the interionic distance R and is characterized by an accuracy that is two orders of magnitude higher than that given by Salpeter and Van Horn [Astrophys. J. **155**, 183 (1969)]. As an application of these results we have considered extremely high-density plasmas characterized by the coexistence between a fluid and a Wigner bcc crystal. In particular, we have shown that the screening potential obtained on the basis of the short-range-order effect, the Widom series expansion, and the lattice calculation near the equilibrium distance is in close agreement with recent Monte Carlo simulations.
[S1063-651X(98)05503-2]

PACS number(s): 52.25.−b, 31.15.−p, 32.70.−n

I. INTRODUCTION

The knowledge of screening potentials is connected with outstanding problems in astrophysics such as the enhancement factor for thermonuclear reaction rates in stellar interiors [1,2]. More recently, renewed interest has been mainly stimulated by experiments where high-power laser beams produce plasmas with an electron density as high as 10^{24} cm^{-3}. To this end, the use of quadrupled laser frequency [3] and the conversion of the laser light into soft-x-ray pulses [4] are the two most efficient methods. In such plasmas, screening effects can deeply modify atomic properties [5,6] and induce formation of quasimolecules [7–9]. In addition, because of its frequent occurrence in entangled numerical codes concerning the most important problems in dense plasmas such as equilibrium rate equations and line broadening, the screening potential needs to be expressed in a simple form with a clear physical meaning for characteristic parameters. Outside the validity domain of the Debye-Hückel theory, the most reliable data for screening potential V_S have been deduced from Monte Carlo computations [10–14] of the radial distribution function

$$g=\exp\left[-\Gamma\left(\frac{a}{R}-h\right)\right], \tag{1}$$

where R is the distance between two given reacting ions, $\Gamma=(Ze)^2/akT$, $a=(3/4\pi n)^{1/3}$, and n are the coupling parameter, the ion-sphere radius, and the ion density, respectively. In Eq. (1), h is the screening potential in units of $(Ze)^2/a$, already used in Ref. [15]:

$$V_S=\frac{(Ze)^2}{a}\,h. \tag{2}$$

By analyzing the results of Brush, Shalin, and Teller [10], De Witt, Grabosk, and Cooper [16] found empirically that outside the zero-separation region and for $\Gamma>1$, h can be accurately expressed in the linear form

$$h_L=C_0-C_1\,\frac{R}{a}, \tag{3}$$

where the coefficients C_0 and C_1 depend slightly on Γ and satisfy the relationship

$$C_0-2\sqrt{C_1}=0. \tag{4}$$

It is remarkable [16,17] that Eqs. (3) and (4) fit the one-component Monte Carlo data as well as the two-component ones.

In our previous works [7,8] we have suggested a two-ion center model for studying the electronic bound states of quasimolecules in high-density plasmas. In particular, possibly different spectral components and a drastic reduction in Stark shifts have been pointed out. Indeed, this screening effect is complete when the interionic distance reaches the value $1.70a$. In the present paper we intend to evaluate the screening potential in extremely high-density plasmas. To this end, lattice sums including 10^9 ions are performed in order to obtain the potential energy as a function of R in Sec. II. An analytical form for the screening potential in plasmas is then given in Sec. III, where general properties of fluids [18] and continuity conditions with respect to the screening potential in lattices are systematically used. This analytical form is proved to be in close agreement with Monte Carlo computations [14]; it is especially useful for examining how quasimolecules are formed and what their effect on spectral line shapes is when spectroscopic diagnostics are performed for the ablation layers of solid targets irradiated by intense laser beams [3]. Also a discussion will be made about its discrepancy in comparison with the pioneering result [1], which is based on the harmonic-oscillator potential in lattices.

II. SCREENING POTENTIAL IN LATTICES

Consider first the ''static lattice approximation'' in which only two nearest-neighboring ions 1 and 2 move. Their relative position vector changes from the equilibrium vector $\vec{R}_{12}$

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to the final one $\vec{R}$ while all other ions plus the center of mass of the reacting pair are ''frozen'' at their initial position. The screening potential is obtained by equating the effective potential $(Ze)^2/R - V_S$ to the energy change of the whole system when the reacting ions move. Then, by taking into account the lattice symmetry, this screening potential can be written in units of $(Ze)^2/a$ as

$$h^{(\mathrm{SL})} = \frac{a}{d}\left[1 + 2\left(\frac{d}{|\vec{R}_{12} - \vec{\nu}/2|} - 1\right) - \theta_0\,\frac{\vec{\nu}^2}{d^2} - S\,\frac{d}{b}\right], \qquad (5)$$

where $d = |\vec{R}_{12}|$, $\vec{\nu} = \vec{R}_{12} - \vec{R}$, and $\theta_0 = d^3/4a^3$. In addition to the ion-sphere radius a and the nearest-neighbor distance d, we have introduced the lattice constant b. For the body-centered-cubic (bcc) and simple cubic lattice we recall the relationship $d = b\sqrt{3}/2 = (\pi\sqrt{3})^{1/3}a$ $(=1.7589a)$ and $d = b = (4\pi/3)^{1/3}a$ $(=1.612a)$, respectively. The second term on the right-hand side of Eq. (5) can be understood as resulting from the interaction of each ion of the interacting pair with the neutralizing background of the other. The third term is due to the background restoring force and the last one $-Sd/b$ comes from the reaction of all surrounding ions when ion 1 or 2 leaves its equilibrium position. Here S is a very symmetric lattice sum, which depends on the lattice structure according to

$$S = 2b\sum_{i\neq 1}\left(\frac{1}{|\vec{R}_{1i} - \vec{\nu}/2|} - \frac{1}{|\vec{R}_{1i}|}\right). \qquad (6)$$

We note that the reduction of the effective potential to its anisotropic harmonic-oscillator term [Eq. (10) in Ref. [1]] can be obtained by adopting $S \equiv 0$ in Eq. (5). For going beyond this second-order approximation, we express $\vec{R}_{1i}$ and $\vec{\nu}$ in terms of the lattice unit vectors $\vec{e}_1$, $\vec{e}_2$, and $\vec{e}_3$, i.e.,

$$\vec{R}_{1i} = \frac{b}{2}\,(p_{i1}\vec{e}_1 + p_{i2}\vec{e}_2 + p_{i3}\vec{e}_3) \qquad (7)$$

and

$$\vec{\nu} = \vec{R}_{12} - \vec{R} = b(c_1\vec{e}_1 + c_2\vec{e}_2 + c_3\vec{e}_3), \qquad (8)$$

and perform the lattice sum (6) over all ions i with reduced coordinates $(p_{i1}, p_{i2}, p_{i3}) \neq (0,0,0)$. In addition, when Γ increases up to $\Gamma_{\mathrm{bcc}} = 172$, dense plasmas freeze first into bcc configuration [19] and consequently p_{i1}, p_{i2}, p_{i3} in Eq. (7) are all even or odd integers. We point out the useful relationships

$$S(-\vec{\nu}) = S(\vec{\nu}) \qquad (9)$$

and

$$S(\vec{\nu}) + \frac{\pi}{2}\left(\frac{\vec{\nu}}{d}\right)^2 + \frac{8d}{\sqrt{3}|\vec{\nu}|} = S(2\vec{R}_{12} - \vec{\nu}) + \frac{\pi}{2}\left(\frac{2\vec{R}_{12} - \vec{\nu}}{d}\right)^2 + \frac{8d}{\sqrt{3}|2\vec{R}_{12} - \vec{\nu}|}, \qquad (10)$$

which we can verify by using the lattice symmetry in Eq. (6) and the fact that the screening potential (5) does not change when we permute the positions of the reacting ions.

A way for improving the harmonic-oscillator approximation consists in starting from the multipole expansion of Eq. (6) and arranging conveniently the ions in spherical shells. In particular, we have shown that the quadrupole term cancels while the hexadecapole one is given by

$$S(\vec{\nu}) = \frac{7\sigma}{12}\,[3c^4 - 5(c_1^4 + c_2^4 + c_3^4)] + O(c^6), \qquad (11)$$

where $c = |\vec{\nu}|/b$ and the numerical factor $\sigma = 3.328\,359 \times 10^{-1}$ has been deduced from a lattice sum over 10^9 ions. To our knowledge, the fourth-order result given in Eq. (11) is a new one.

Henceforth, for the comparison purpose with the high-density plasma case, we consider only longitudinal displacements $\vec{\nu} = \xi\vec{R}_{12}$, where $\xi = 1 - R/d$. Equations (9) and (10) show that $S(\xi)$ is an even function of ξ and completely defined by its numerical values for $\xi \in [0,1]$. The lattice sum (6) with $c_1 = c_2 = c_3 = \xi/2$ has been performed by considering $64p_0^3$ $(p_0 = 150)$ nearest ions. The contribution of the far-off ions with $p \geqslant p_0$ is of the order of magnitude of $(a^2/d^2p_0)^2$ and has been included by using a reliable extrapolation process. Finally, we obtain

$$\begin{aligned} S(\xi) = \tfrac{1}{10}\xi^4(&1.456\,157 + 1.276\,584\xi^2 + 5.523\,994\times 10^{-2}\xi^4 \\ &+ 7.218\,356\times 10^{-2}\xi^6 + 2.019\,800\times 10^{-3}\xi^8 \\ &+ 7.140\,663\times 10^{-3}\xi^{10}), \end{aligned} \qquad (12)$$

where the absolute error of the polynomial in parentheses is less than $\pm 3\times 10^{-6}$. We note that the first term in Eq. (12) is in agreement with the hexadecapole approximation (11):

$$S(\xi) = (7\sigma/16)\xi^4 + O(\xi^6).$$

Then, for longitudinal displacements, the screening potential in lattices (5) can be written as

$$h^{(\mathrm{SL})} = \frac{a}{d}\left[1 + \xi - \left(\theta^{(\mathrm{SL})} - \frac{1}{2-\xi}\right)\xi^2\right], \qquad (13)$$

where $\theta^{(\mathrm{SL})} = \theta_0 + S(\xi)(d/b\xi^2)$ expresses that the background restoring effect is amplified by the surrounding frozen ions, which tend to prevent the reacting ions from large displacements. Equation (13) is particularly accurate for $\xi < 1$; its error is indeed less than $1.5\times 10^{-7}\xi^2$ owing to the precision of Eq. (12).

When the variable $\eta = R/d$ is used instead of $\xi = 1 - \eta$, accounting for the symmetry properties in Eqs. (9) and (10), Eq. (13) takes the form

$$h^{(SL)} = \frac{a}{d}\left\{\frac{3+\eta^2}{1-\eta^2} - \frac{\pi\sqrt{3}}{4}\,(1+\eta^2) - \frac{\sqrt{3}}{4}\,[S(1+\eta) + S(1-\eta)]\right\}$$

$$=\left(\frac{1}{\pi\sqrt{3}}\right)^{1/3}(1.391\,160-0.258\,399\,\eta^2 -0.162\,060\,\eta^4+0.034\,887\,\eta^6-0.005\,798\,\eta^8 +0.000\,210\,\eta^{10}), \quad (14)$$

which shows clearly that the screening potential in lattices, like in fluids [18], is an even function of R. Equations (13) or (14) is recommended instead of Eq. (11) in Ref. [1] where the above-mentioned symmetry property is violated and also the error is estimated to be $\pm 2\times 10^{-4}$.

III. SCREENING POTENTIAL IN FLUID PLASMAS

Despite its high accuracy resulting from the very large number of ions considered in lattice sums, we must keep in mind that Eqs. (13) or (14) applies only to small displacements with typically $|\xi|<0.25$. For larger values of $|\xi|$ violating Lindemann's criterion, the static lattice assumption used in Sec. II is no longer valid. On the contrary, the surrounding lattice points tend to polarize into the relaxed positions appropriate to each given distance between the reacting ions $R=(1-\xi)d=\eta d$. With the purpose of generalizing Eq. (13) to short interionic distances, according to Widom's work [18], we can expand the screening potential h in the following power series in R^2:

$$h=\frac{a}{d}\,(a_0-a_1\eta^2+a_2\eta^4-a_3\eta^6+\cdots) =h_0-h_1r^2+h_2r^4-h_3r^6+\cdots\ , \quad (15)$$

where in addition to $\eta=R/d$ we have introduced the variable $r=R/a$ for making easier the comparison with other works [14,15,22].

The coefficients a_k (h_k) in Eq. (15) are all functions of Γ except for a_1, which is $\theta_0=d^3/4a^3=1.3603$ ($h_1=0.25$) according to Eq. (5) and Ref. [20]. The coefficient a_0 is defined by the increment of the chemical potential for the reacting pair before and after the nuclear fusion; its dependence on Γ is weak but very real. Recently, using a different Monte Carlo (MC) method [14], Ogata has obtained accurate $g(R)$ results down to small R. Note, however, that Ogata's values for a_0 are 1% larger than those given by Rosenfeld [15]. In part this is because in Ogata's analysis he uses a fit to one-component plasma fluid energy data U/NkT that is slightly inaccurate in comparison to the more recent ones [21]. Concerning the coefficient a_2, the best available estimate is due to Rosenfeld [15], who considered the continuity between MC results [14] and the three-term series expansion for the amplitude and its first two derivatives. However, it is interesting to note that Rosenfeld's value $a_2=0.52$ ($h_2=0.031$) for $\Gamma=160$ would change to a larger number if he had used a nonzero value of a_3. The latter coefficient has been considered by Alastuey and Jancovici [22], who used the limited MC $g(R)$ data available in 1977 and found $a_2=0.657$ ($h_2=0.039$) and $a_3=0.224$ ($h_3=0.0043$) for $\eta\in[0.00,0.91]$.

In the present work, we will determine the coefficients a_0, a_2, and a_3 in Eq. (15) by using the screening potential in lattices (13) and two characteristic properties of strong-coupling plasmas. The first one concerns $g_{\max}$, which is the amplitude of the first peak of the radial distribution function g and gives a measure of the short-range-order effect. In accordance with MC calculations [11,12] for $\delta=(1/\Gamma)\ln g_{\max}$, we suggest the fit

$$\delta=\left(0.544-0.401\ln\frac{\Gamma}{160}\right)\times 10^{-2},\quad \Gamma\in[140,200]. \quad (16)$$

Denoting by $r_{\max}$ the location of the first peak of g ($g=g_{\max}$, $h=1/r_{\max}+\delta$, and $dh/dr=-1/r_{\max}^2$ for $r=r_{\max}$), the linear form (3) with

$$C_0=\frac{2}{r_{\max}}+\delta,\quad C_1=\frac{1}{r_{\max}^2} \quad (17)$$

is a useful approximation for h in the interval where the second derivative d^2h/dr^2 is small (see Table I). From Eq. (17) we can see that $C_0-2\sqrt{C_1}=\delta$ is in agreement with Eq. (4) in the sense that δ is very small in comparison to C_0. We note that Eq. (17) is free from the restrictive lattice assumption [23] $r_{\max}=d/a$, i.e., $h_L=(a/d)(2-ar/d)$, and consequently applies to plasmas with $\Gamma<\Gamma_{\mathrm{bcc}}$.

The second characteristic property of strong-coupling plasmas consists in a close agreement between h [Eq. (15)] and $h^{(\mathrm{SL})}$ [Eq. (13)] when the latter is valid, i.e., for $\Gamma=\Gamma_{\mathrm{bcc}}=172$ [19] and $|\xi|<0.25$. Indeed, as shown in the Appendix, the discrepancy between h and $h^{(\mathrm{SL})}$ can be written in the form

$$h-h^{(\mathrm{SL})}=(-1)^p\alpha_p(\xi-\xi_0)^p+O(\xi^{p+1}), \quad (18)$$

where ξ_0 is a value of ξ chosen in the allowed interval and α_p, with $p\geqslant 2$, is a linear combination of the coefficients $a_0,a_1,a_2,\ldots,a_p$. In Eq. (18), $O(\xi^{p+1})$ is of the same order of magnitude as ξ^{p+1} and cancels exactly for $\xi=\xi_0$. As a result, we can see that the discrepancy $h-h^{(\mathrm{SL})}$ cancels at $\xi=\xi_0$ and is of the order of magnitude $(\xi-\xi_0)^p$ or ξ^{p+1} for $\xi\neq\xi_0$. In addition, there are p conditions that underlie Eq. (18) and give $a_0,a_1,a_2,\ldots,a_p$ as functions of ξ_0. For the purpose of a comparison with available data we consider principally the case $p=3$, i.e., the series expansion (15) truncated at the fourth term. In Table I we give the coefficients a_0,a_2,a_3 of the screening potential h and those C_0,C_1 of the related linear approximation h_L [Eqs. (3) and (17)] as functions of the distance $R_0=\eta_0 d/a$, which corresponds to the best agreement between $h(\eta)$ and $h^{(\mathrm{SL})}(\eta)$ in accordance with Eq. (18). A careful examination of Table I shows that $\delta=C_0-2\sqrt{C_1}=(1/\Gamma)\ln g_{\max}$ is the only parameter really sensitive to a variation of η_0. Indeed, when η_0 increases from 1.1500 to 1.1790, we note that δ increases by 62% while, for example, a_0 increases only by 0.84%. This sensitive variation of the constant of the short-range-order effect δ is useful for selecting the suitable joining point η_0 between the fluid (h) and lattice ($h^{(\mathrm{SL})}$) screening potential.

The most direct application of our present calculation consists of considering the coupling parameter $\Gamma=172$, which characterizes the coexistence between a Wigner bcc crystal and a fluid plasma [19]. Equation (16) gives $\delta d/a=0.906\times 10^{-2}$ and supports the choice $\eta_0=1.1617$ and the

TABLE I. Screening potential parameters for plasmas in liquid-crystal equilibrium. Here δ', C_0', and C_1' denote $(d/a)\delta$, $(d/a)C_0$, and $(d/a)^2C_1$, respectively. Likewise, the relationship $a_k=(d/a)^{2k+1}h_k$ $(k=0,1,2,3)$ is to be used for deducing h_k from a_k in Eqs. (15) and (19). We note that the constant of short-range-order effect $\delta=(1/\Gamma)\ln g_{\max}=C_0-2\sqrt{C_1}$ [see Eqs. (17)] is consistent with Monte Carlo data [Eq. (16) with $\Gamma=172$] provided the value $\eta_0=1.1617$ and those in the corresponding third column are adopted. The last column is given for referring to the Salpeter and Van Horn's constant $a_0=a_0^{(\mathrm{SVH})}=1.8597$ $(h_0=1.0573)$.

point of maximum agreement between h and $h^{(\mathrm{SL})}$	$\eta_0=1.1500$	1.1560	1.1617	1.1700	1.1790
coefficient of agreement between h and $h^{(\mathrm{SL})}$	$-\alpha_3=1.3003$	1.2684	1.2391	1.1988	1.1571
coefficients of Widom's series expansion ($a_1=\theta_0=1.3603$)	$a_0=1.8443$	1.8474	1.8505	1.8549	1.8597
	$a_2=0.7493$	0.7442	0.7393	0.7326	0.7256
	$a_3=0.2274$	0.2248	0.2223	0.2190	0.2155
location and slope at the inner inflection point	$\eta_-=0.6860$	0.6893	0.6925	0.6970	0.7019
	$m_-=1.1061$	1.1104	1.1144	1.1201	1.1263
location and slope at the outer inflection point	$\eta_+=0.9207$	0.9216	0.9223	0.9234	0.9243
	$m_+=1.0683$	1.0740	1.0793	1.0869	1.0951
parameters of the linear approximation	$\eta_{\max}=0.9647$	0.9625	0.9603	0.9572	0.9539
	$C_1'=1.0746$	1.0795	1.0843	1.0914	1.0991
	$C_0'=2.0806$	2.0786	2.0917	2.0997	2.1087
	$100\delta'=0.7364$	0.0082	0.9060	1.0384	1.1957

corresponding third column in Table I. So we can write the screening potential (15) and the related linear approximation (3) in the form

$$h=\left(\frac{1}{\pi\sqrt{3}}\right)^{1/3}(1.8505-\theta_0\eta^2+0.7393\eta^4-0.2223\eta^6)$$
$$=1.0521-0.25r^2+0.043\,92r^4-0.004\,269r^6,$$
$$r\in[0.0,2.0] \qquad (19)$$

and

$$h_L=\left(\frac{1}{\pi\sqrt{3}}\right)^{1/3}(2.0917-1.0843\eta)=1.1892-0.3505r, \qquad (20)$$

respectively. We note that the first peak of the radial distribution function is located at the distance $R_{\max}/a=(\eta_{\max}d)/a=1.6891$, which is appreciably shorter than the nearest-neighbor distance in the lattice $d/a=1.7589$. In addition to the values 1.0843, 1.0793, and 1.1144 of the derivative $dh/d\eta$ at $\eta_{\max}=0.9603$, the outer $(\eta_+=0.9223)$ and inner $(\eta_-=0.6925)$ inflection points are the signature of the agreement between Eqs. (19) and (20) over a large interval approximately equal to $[0.40,\eta_{\max}]$.

In comparison with Alastuey and Jancovici's results [22], we note a good agreement for a_3 and a discrepancy of 11% for a_2. Another difference consists in the validity interval of r, which is [0.0,2.0] for Eq. (19) instead of [0.0,1.6] for Eq. (24) in Ref. [22].

Nevertheless, the most appropriate comparison we would make consists of considering Ogata, Iyetomi, and Ichimaru's work [14] where relative motions of neighboring sites in the bcc lattices have been analyzed through the Monte Carlo sampling method. These authors have given

$$h^{(\mathrm{OII})}=\begin{cases}1.1830-0.3500r+\dfrac{1}{r}\exp(13.2\sqrt{r}-22.1), & r\in[0.7,2.0]\\ 1.0605-0.25r^2, & r\in[0.0,0.7].\end{cases} \qquad (21)$$

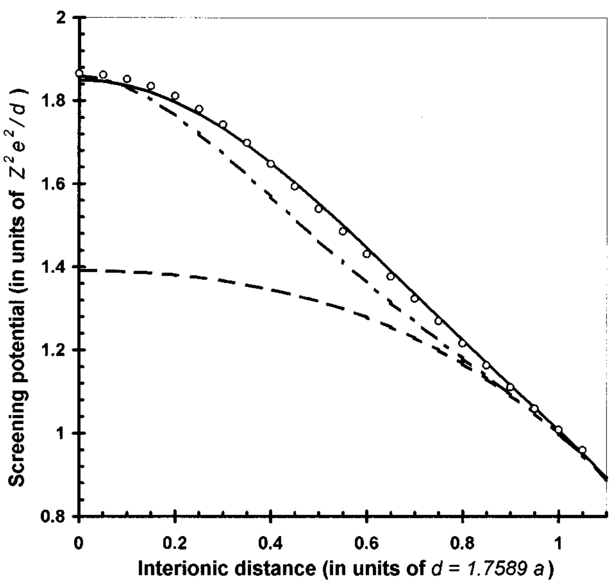

FIG. 1. Screening potential of plasmas in liquid-crystal equilibrium. We note that the present theory leading to $h(\eta)$(——), Eq. (19), is in close agreement with Monte Carlo simulations [14], $h^{(\mathrm{OII})}(\eta)$ (○○○), especially in the interval $\eta \in [0.3,1.10]$. The discrepancy between $h(\eta)$ and the lattice screening potential (–––), Eq. (13), increases rapidly outside the joining zone ($\eta<0.9$). The Salpeter and Van Horn's screening potential $h^{(\mathrm{SVH})}(\eta)$(–·–) is smaller than $h(\eta)$ and $h^{(\mathrm{OII})}(\eta)$ by 6%.

It is interesting to note that the coefficients $C_0-\delta=1.1840$ and $C_1=0.3505$ in Eq. (20) are in agreement with those of the linear part in Eq. (21). Indeed, Fig. 1 shows that our analytical result (19) and the Monte Carlo results are in very good agreement, in particular in the interval $r\in[0.7,2.0]$, where the discrepancy between h [Eq. (19)] and its linear approximation h_L [Eq. (20)] is less than 0.5%. Concerning the agreement between h and $h^{(\mathrm{SL})}$ in the vicinity of the equilibrium position, Fig. 1 and a numerical check show that $100(1-h^{(\mathrm{SL})}/h)$ decreases from 0.7 to -0.4 when η increases from 1 to 1.20. This results in fact from the condition $h-h^{(\mathrm{SL})}\approx-\alpha_3(\eta-1.1617)^3$ occurring in Eq. (18).

In comparison with the screening potential resulting from the pioneering relaxed lattice model of Salpeter and Van Horn [Eq. (14) in Ref. [1]]:

$$h^{(\mathrm{SVH})}=\left(\frac{1}{\pi\sqrt{3}}\right)^{1/3}(1.8597-3.0439\eta^2+3.6540\eta^3-1.4697\eta^4), \tag{22}$$

we mention the following differences:

(i) For the reference potential at $\eta\approx1$, the harmonic-lattice potential is used in Eq. (22) instead of the more accurate one [Eqs. (13) or (14) given in Sec. I]. In addition, the linear approximation for $h^{(\mathrm{SVH})}$ and $\eta\approx1$ results directly from that of the static-lattice potential $h_L^{(\mathrm{SL})}=(a/d)(2-\eta)$, while Eq. (20) has been deduced self-consistently by considering the maximum of the radial distribution.

(ii) The right-hand side of Eq. (22) is not an even function of η [18]. This violation of symmetry is also observed in the static-lattice model [Eq. (11) in Ref. [1]]. [See Eq. (14) and related comments of the present work.]

(iii) In Eq. (22) the term due to background restoring forces $-3.0439\eta^2$ is too large in comparison to the exact one $-\theta_0\eta^2$ ($\theta_0=1.3603$).

In a large interval of intermediate values of η, Fig. 1 shows that $h^{(\mathrm{SVH})}$ is 6% smaller than our calculated h [Eq. (19)] and Monte Carlo's results [14].

In a more recent work [23], $h^{(\mathrm{SVH})}$ has been modified in such a way to involve the exact background force effect $-\theta_0\eta^2$. Nevertheless, the improvement is not really conclusive because conditions (i) and (ii) have not been taken into account.

IV. CONCLUSION

This paper is concerned with the screening potential (SP) of extremely high-density plasmas that occur in stellar objects such as white dwarfs [1] and also in laboratory experiments such as ablation of crystal targets when the latter are irradiated by intense and short-wavelength laser beams. Concerning the SP in lattices, we have shown that the harmonic-oscillator approximation can be improved by introducing the hexadecapole term, which has been calculated by means of a suitable association of ionic points in spherical shells. This term is in agreement with the lattice sums performed for arbitrarily large longitudinal displacements and 10^9 nearest ionic points. The present SP in lattices is, like in fluids, an even function of R and is characterized by an accuracy that is of two orders of magnitude higher than that of Eq. (11) in Ref. [1]. It is the basis of the joining process leading to a precise SP $h(\eta)$ that proves to be very close to the one given by Monte Carlo simulations [14]. Concerning the linear form $h_L=C_0-C_1r$ exhibited in most Monte Carlo simulations, we have shown that the relationship $C_0\approx2\sqrt{C_1}$ merely results from the fact that h_L is a common linear approximation for the ''augmented Coulomb potential'' $h_c=1/r+\delta$ and the SP h of which the second derivative is very small for $R\neq0$. This relationship is discussed in terms of the short-range-order effect $\delta(\Gamma)$ instead of the harmonic oscillations in lattices and is valid for a large range of Γ down to $\Gamma\approx2$ with $\delta\approx0$.

To obtain an accurate closed form for the SP, which is necessary to many numerical codes (population rates, line broadening, formation of transient molecules, etc.), it is useful to generalize the present joining method to other plasma conditions. Also, when the two reacting ions are very close, corrections due to bound electron quantum effects [7] and free-electron inhomogeneity [7,8] are to be introduced.

APPENDIX: SOLUTION FOR THE JOINING PROBLEM BETWEEN SCREENING POTENTIALS IN LATTICES AND IN FLUID PLASMAS

With the purpose of joining the screening potential in fluid plasmas with that in static lattices we write their discrepancy in the form

$$h=h^{(\mathrm{SL})}=\alpha_0-\alpha_1\xi+\alpha_2\xi^2-\alpha_3\xi^3+\cdots+(-1)^p\alpha_p\xi^p+O(\xi^{p+1}), \tag{A1}$$

where, according to Eqs. (13) and (15), $\alpha_0, \alpha_1, \ldots, \alpha_p$ are linear combinations of $a_1 = \theta_0$ and unknown coefficients $a_0, a_2, a_3, \ldots, a_p$,

$$\alpha_0 = -(1+\theta_0 - a_0) + a_2 - a_3 + a_4 + \cdots + (-1)^p a_p,$$

$$\alpha_1 = -(2\theta_0 - 1) + 4a_2 - 6a_3 + 8a_4 + \cdots + (-1)^p \frac{2p}{1!} a_p,$$

$$\alpha_2 = -\frac{1}{2} + 6a_2 - 15a_3 + 28a_4 + \cdots + (-1)^p \frac{2p(2p-1)}{2!} a_p,$$

$$\alpha_3 = \frac{1}{4} + 4a_2 - 20a_3 + 56a_4 + \cdots + (-1)^p \frac{(2p)!}{(2p-3)!3!},$$

$$\alpha_4 = 0.001\,107 + a_2 - 15a_3 + 70a_4 + \cdots + (-1)^p \frac{(2p)!}{(2p-4)!4!} a_p. \quad \text{(A2)}$$

In Eq. (A1), $O(\xi^{p+1})$ is of the same order of magnitude as ξ^{p+1}. Here we note that for a given value ξ_0, Eq. (A1) can take the form of Eq. (18) in the text, provided the $p-1$ following conditions are ensured:

$$\frac{d^i}{d\xi^i}[\alpha_0 - \alpha_1 \xi + \alpha_2 \xi^2 - \cdots + (-1)^p \alpha_p \xi^p] = 0$$

$$\text{for } \xi = \xi_0, \quad \text{all } i \in [1, p-1]. \quad \text{(A3)}$$

By taking into account Eq. (A2), these conditions allow us to determine $a_2, a_3, \ldots, a_p$ as functions of ξ_0. To finish solving the problem, we require that for $\xi = \xi_0$, $O(\xi^{p+1}) = 0$, i.e.,

$$h - h^{(\mathrm{SL})} = 0. \quad \text{(A4)}$$

Equation (A4), together with Eqs. (13) and (15) in the main text, serves to express a_0 in terms of $\xi_0, a_2, a_3, \ldots,$ and a_p. For $p=3$ in particular we have

$$a_2 = \frac{1}{\Delta}\left[\frac{5\theta_0 - 3}{2} - 10\left(\theta_0 - \frac{37}{80}\right)\xi_0 + \frac{55}{16}\xi_0^2\right],$$

$$a_3 = \frac{1}{\Delta}\left[\theta_0 - \frac{2}{3} - 2\left(\theta_0 - \frac{3}{8}\right)\xi_0 + \frac{7}{8}\xi_0^2\right],$$

$$\Delta = 2 - 14\xi_0 + 15\xi_0^2, \quad \text{(A5)}$$

while Eq. (A4) results in

$$a_0 = h^{(\mathrm{SL})}(\xi_0) + \theta_0(1-\xi_0)^2 - a_2(1-\xi_0)^4 + a_3(1-\xi_0)^6,$$

$$\alpha_3 = \tfrac{1}{4} + 4a_2 - 20a_3. \quad \text{(A6)}$$

For suitable values of $\eta_0 = 1 - \xi_0$, the coefficients in Eqs. (A5) and (A6) are given in Table I.

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