Temperature-dependent pseudopotential between two pointlike electrical charges

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Pair distribution functions for particles electrically charged, at a temperature T expressed in terms of density matrices and corresponding pseudopotentials are studied, for distinguishable particles and for an electron pair. Expansions with respect to the separation distance and to a quantum parameter ($\sim T^{-1/2}$) are carried out. Approximate expressions are derived in the limits of high and low temperatures.

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I. INTRODUCTION

Some years ago, Gombert and co-workers studied the pseudopotential $V_{ij}(r)$ between two pointlike electrical charges at a temperature T [1,2]. More precisely, they evaluated the pair distribution function, which is expressed in terms of density matrices as

$$g_{ij}(r)=\exp[-\beta V_{ij}(r)]=\frac{\rho_2(\mathbf{x}_i,\mathbf{y}_j,\mathbf{x}_i,\mathbf{y}_j,\beta)}{\rho_1(\mathbf{x}_i,\mathbf{x}_i,\beta)\rho_1(\mathbf{y}_j,\mathbf{y}_j,\beta)}, \tag{1}$$

with $\beta=1/k_BT$ and $r=|\mathbf{x}_i-\mathbf{y}_j|$. i and j refer to the particle species. $\mathbf{x}_i$ and $\mathbf{y}_j$ are the particle positions. ρ_1 and ρ_2 are the one- and two-particle density matrices, respectively. There is a temperature, but no account is taken of the other particles in the plasma (no screening). It is a way to represent the quantum effects at a small separation distance r. In the case where r is much greater than the de Broglie length $\lambda\!\!\!^{-}_{ij}$ $[=\hbar(k_BT\mu_{ij})^{-1/2}$ in which μ_{ij} is the reduced mass of the pair of particles], $V_{ij}(r)$ reduces to the Coulomb potential.

For undistinguishable particles, the symmetry of the wave functions has to be taken into account. In the case of two electrons, the pair distribution function is

$$g_{ee}(r)=\exp[-\beta V_{ee}(r)]$$
$$=\frac{\rho_2(\mathbf{x},\mathbf{y},\mathbf{x},\mathbf{y},\beta)-\frac{1}{2}\rho_2(\mathbf{x},\mathbf{y},\mathbf{y},\mathbf{x},\beta)}{\rho_1(\mathbf{x},\mathbf{x},\beta)\rho_1(\mathbf{y},\mathbf{y},\beta)}. \tag{2}$$

At high temperature, i.e., in the case where the Landau length ($=|Z_iZ_j|e^2\beta$, Z_ie and Z_je being the two electrical charges which can be positive or negative) is smaller than $\lambda\!\!\!^{-}_{ij}$, some simple expressions to approach $V_{ij}(r)$ have been proposed [1,2].

In this paper, expansions of g_{ij} are carried out. There are two expansion parameters, $x(=r/\lambda\!\!\!^{-}_{ij})$ and a quantum parameter ξ:

$$\xi=-Z_iZ_je^2\beta/\lambda\!\!\!^{-}_{ij}\sim T^{-1/2}, \tag{3}$$

which can be positive or negative. From this study, approximate expressions for $V_{ij}(r)$ are also derived in the cases of high and low temperatures. Section II is devoted to a pair of distinguishable particles and Sec. III to the electron pair.

This work is following the studies performed first by Kelbg who calculated exactly $V_{ee}^{no\ exc}(r)$, the pseudopotential for an electron pair without taking account of the exchange between the two electrons, for very high temperature ($|\xi|\to 0$) [3], then by Davies and Storer who studied completely the case of zero separation and wrote expansions with respect to a quantum parameter related to ξ [4]. Rohde *et al.* [5] expressed the binary Slater sums (i.e., g_{ij} or g_{ee}) as expansions with respect to r and proposed approximations. Numerical calculations were done by other authors: Storer [6], Barker [7]. Let us mention other pioneers in this field who are Trubnikov and Elesin [8]. More recently, Vieillefosse also worked on this topic [9].

These potentials are made to be used, in the framework of classical statistical mechanics, in order to evaluate thermodynamical quantities in a plasma as was done, for instance, by Kelbg and co-workers [10,11] and later by Deutsch and co-workers [12–17], who proposed simple forms to approach these potentials [1] and used these simple approximations. They were also used by other authors to deal with transport problems [18,19] or with thermodynamical properties of dense plasmas at high temperature [20]. As the quantum mechanics is introduced via a two-body potential, it is a way to study plasma properties, which is not valid if the density is too high. This way, quantum corrections to the classical properties can be evaluated. These potentials are finite at the origin [4]. Thus, this method permits to avoid the divergence which appears in the classical studies of plasmas (with both charge signs). We remark that, at high temperature ($|Z_iZ_j|e^2\beta<\lambda\!\!\!^{-}_{ij}$), it is necessary to introduce quantum corrections in order to study the properties of a plasma.

II. DISTINGUISHABLE PARTICLES

Let

$$g_{ij}(r)=\begin{cases} g_{ij}^s(r)+g_{ij}^b(r) & \text{for unlike charge signs,}\\ g_{ij}^s(r) & \text{for like charge signs,}\end{cases} \tag{4}$$

where $g_{ij}^b(r)$ is the contribution due to the bound states and $g_{ij}^s(r)$ is that due to the scattering states.

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A. Scattering state contribution, g_{ij}^s

$g_{ij}^s(r)$ can be written as follows:

$$g_{ij}^s(r)=\int \frac{d^3k}{(2\pi)^3}\exp\left(-\frac{\hbar^2k^2\beta}{2\mu_{ij}}\right)\frac{1}{4\pi}\int_0^{2\pi}d\varphi \times\int_0^{\pi}d\theta\sin(\theta)\Psi_C\Psi_C^* \Bigg/ \int\frac{d^3k}{(2\pi)^3}\exp\left(-\frac{\hbar^2k^2\beta}{2\mu_{ij}}\right) = \frac{\lambda_{ij}^3}{(2\pi)^{1/2}}\int_0^{\infty}dk\,k^2\exp\left(-\frac{1}{2}\lambda_{ij}^2k^2\right)\int_{-1}^{+1}du\,\Psi_C\Psi_C^*. \tag{5}$$

Ψ_C is the Coulomb wave function [21]:

$$\Psi_C=\exp(-\alpha\pi/2)\Gamma(1+\mathrm{i}\alpha)\exp(ikru) \times{}_1F_1(\mathrm{i}\alpha,1;-\mathrm{i}k(r-ru)), \tag{6}$$

where $\alpha=Z_iZ_je^2\beta/\lambda_{ij}^2k$, $u=\cos\theta$, and θ is the angle $(\mathbf{r},\mathbf{k})$. ${}_1F_1$ is the confluent hypergeometric function. Expressing Ψ_C, g_{ij}^s becomes

$$g_{ij}^s(r)=(2\pi)^{1/2}\lambda_{ij}^3\int_0^{\infty}dk\,k^2\alpha\frac{\exp\left(-\frac{1}{2}\lambda_{ij}^2k^2\right)}{\exp(2\pi\alpha)-1} \times\int_0^2 dv\,{}_1F_1(-\mathrm{i}\alpha,1;\mathrm{i}krv)\,{}_1F_1(\mathrm{i}\alpha,1;-\mathrm{i}krv). \tag{7}$$

Making use of the dimensionless quantities $K=|2\alpha|^{-1}=k\lambda_{ij}/2|\xi|$ and $x=r/\lambda_{ij}$, the last equation is rewritten in the form

$$g_{ij}^s(x)=-8(2\pi)^{1/2}\xi^3\int_0^{\infty}dK\,K\frac{\exp(-2\xi^2K^2)}{\exp(\epsilon\pi/K)-1}A, \tag{8}$$

with

$$\epsilon=-|\xi|/\xi \tag{9}$$

and

$$A=\frac{1}{2}\int_0^2 dv\,{}_1F_1\left(-\frac{\epsilon i}{2K},1;2i|\xi|Kxv\right) \times{}_1F_1\left(\frac{\epsilon i}{2K},1;-2i|\xi|Kxv\right). \tag{10}$$

A has been expanded in increasing powers of K^2 with the result

$$A=\sum_{p=0}^{\infty}(-1)^p(4\xi Kx)^{2p}\sum_{q=0}^{\infty}C(p,q)(-2\xi x)^q. \tag{11}$$

$C(p,q)$, in which p and q are integers, is a number defined as

$$C(p,q)=\frac{1}{2p+q+1}\sum_{n=0}^{2p}(-1)^n \times\sum_{m=0}^{q}\frac{\mathcal{S}_{m+n}^{(m)}\mathcal{S}_{q-m+2p-n}^{(q-m)}}{[(m+n)!(q-m+2p-n)!]^2}, \tag{12}$$

where $\mathcal{S}_m^{(n)}$ $(n\leqslant m)$ are the Stirling numbers of the first kind [22]. Note that

$$C(p,0)=\delta_{p0}\quad\text{and}\quad C(0,q)=\frac{(2q)!}{(q+1)!(q!)^3}. \tag{13}$$

Then, $g_{ij}^s(x)$ is put in a form involving p derivatives with respect to ξ^2 as follows:

$$g_{ij}^s(x)=g_{ij}^s(0)-8(2\pi)^{1/2}\xi^3 \times\sum_{p=0}^{\infty}\left(\frac{2^pd^p}{d(\xi^2)^p}\int_0^{\infty}\frac{dK\,K\exp(-2\xi^2K^2)}{\exp(\epsilon\pi/K)-1}\right) \times\sum_{q=1}^{\infty}C(p,q)(-2\xi x)^{2p+q}. \tag{14}$$

The integral over K is known, it was evaluated by Davies and Storer in the calculation of $g(0)$. Thus,

$$g_{ij}^s(x)=g_{ij}^s(0)+\xi^3\sum_{p=0}^{\infty}\left[\left(\frac{1}{\xi}\frac{d}{d\xi}\right)^p[\xi^{-3}g_{ij}^s(0)]\right] \times\sum_{q=1}^{\infty}C(p,q)(-2\xi x)^{2p+q}, \tag{15}$$

where [4]

$$g_{ij}^s(0)=1+(2\pi)^{1/2}\xi+\sum_{k=0}^{\infty}(-1)^k\frac{2^{k/2+1}}{k!}\Gamma\left(\frac{k}{2}+1\right) \times\zeta(k+2)|\xi|^{k+2}. \tag{16}$$

$\zeta(n)$ are Riemann's ζ functions. Therefore, Eq. (15) becomes

$$g_{ij}^s(x)=\sum_{p=0}^{\infty}(-8x^2)^p\Bigg[(3/2)_p+p!(2\pi)^{1/2}\xi +\sum_{k=0}^{\infty}(-1)^k\frac{2^{k/2+1}}{k!}\Gamma\left(\frac{k}{2}+1\right)\zeta(k+2) \times\left(\frac{1-k}{2}\right)_p|\xi|^{k+2}\Bigg]\sum_{q=0}^{\infty}C(p,q)(-2\xi x)^q. \tag{17}$$

B. Bound state contribution, g_{ij}^b

Now we are interested in g_{ij}^b, the part of the pair distribution function due to the bound states. It reads

$$g_{ij}^{b}(r)=(2\pi)^{3/2}\lambda_{ij}^{3}\sum_{n=1}^{\infty}\sum_{\ell=0}^{n-1}\sum_{m=-\ell}^{+\ell}\exp(-\beta E_n)\times\frac{1}{4\pi}\int_0^{2\pi}d\varphi\int_0^{\pi}d\theta\sin\theta\Psi_{n\ell m}(r,\theta,\varphi)\Psi_{n\ell m}^{*}(r,\theta,\varphi). \tag{18}$$

$\Psi_{n\ell m}$ and E_n are the wave functions and the energies of bound states corresponding to the quantum numbers n, ℓ, and m [21]. Expressing them, the last equation becomes

$$g_{ij}^{b}(r)=2(2\pi)^{1/2}\frac{\lambda_{ij}^{3}}{a^3}\sum_{n=1}^{\infty}\frac{1}{n^4}\exp\left(-\frac{2r}{na}-\beta E_n\right)\times\sum_{\ell=0}^{n-1}(2\ell+1)(n-\ell-1)!(n+\ell)!\times\left[\sum_{k=0}^{n-\ell-1}\frac{(-2r/na)^{\ell+k}}{(n-\ell-k-1)!(2\ell+k+1)!k!}\right]^2, \tag{19}$$

with $E_n=Z_iZ_je^2/(2an^2)$ and $a=\hbar^2/(\mu_{ij}|Z_iZ_j|e^2)$. Hence,

$$g_{ij}^{b}(x)=2(2\pi)^{1/2}\xi^3\sum_{n=1}^{\infty}\frac{1}{n^4}\exp\left(\frac{\xi^2}{2n^2}-\frac{2}{n}\xi x\right)\times\sum_{\ell=0}^{n-1}(2\ell+1)(n-\ell-1)!(n+\ell)!\times\left[\sum_{k=0}^{n-\ell-1}\frac{(-2\xi x/n)^{\ell+k}}{(n-\ell-k-1)!(2\ell+k+1)!k!}\right]^2, \tag{20}$$

where $x=r/\lambda_{ij}$. In this case, ξ is positive. $g_{ij}^{b}(x)$ can be expanded with respect to x and ξ, with the result

$$g_{ij}^{b}(x)=g_{ij}^{b}(0)+2(2\pi)^{1/2}\xi^3\times\sum_{p=1}^{\infty}\sum_{k=0}^{\infty}\frac{\zeta(2k+2p+3)}{2^k k!}\xi^{2k}\sum_{q=1}^{\infty}C(p,q)\times(-2\xi x)^{2p+q}. \tag{21}$$

$C(p,q)$ is the number defined by Eq. (12). In the last equation, the sum over k can be rewritten in order to introduce $g_{ij}^{b}(0)$,

$$\sum_{k=0}^{\infty}\frac{\zeta(2k+2p+3)}{2^k k!}\xi^{2k}=\frac{2^{p+1}}{\pi^{1/2}}\frac{d^p}{d(\xi^2)^p}\sum_{k=0}^{\infty}2^k\frac{\Gamma\left(k+\frac{3}{2}\right)}{(2k+1)!}\zeta(2k+3)\xi^{2k}. \tag{22}$$

Making use of the expansion of $g_{ij}^{b}(0)$ [4], $g_{ij}^{b}(x)$ is then expressed in the form

$$g_{ij}^{b}(x)=g_{ij}^{b}(0)+\xi^3\sum_{p=0}^{\infty}\left[\left(\frac{1}{\xi}\frac{d}{d\xi}\right)^p[\xi^{-3}g_{ij}^{b}(0)]\right]\times\sum_{q=1}^{\infty}C(p,q)(-2\xi x)^{2p+q}. \tag{23}$$

C. General expansion of g_{ij}

Equations (15) and (23) are very similar. Thus $g_{ij}(x)$ can be written as

$$g_{ij}(x)=g_{ij}^{s}(x)+\frac{1-\epsilon}{2}g_{ij}^{b}(x)=g_{ij}(0)+\xi^3\sum_{p=0}^{\infty}\left[\left(\frac{1}{\xi}\frac{d}{d\xi}\right)^p[\xi^{-3}g_{ij}(0)]\right]\times\sum_{q=1}^{\infty}C(p,q)(-2\xi x)^{2p+q}. \tag{24}$$

The expansion of $g_{ij}(0)$ is

$$g_{ij}(0)=1+(2\pi)^{1/2}\xi+\sum_{k=0}^{\infty}\frac{2^{k/2+1}}{k!}\Gamma\left(\frac{k}{2}+1\right)\zeta(k+2)\xi^{k+2}. \tag{25}$$

Therefore, the explicit expansion of $g_{ij}(x)$ with respect to x and ξ [corresponding to Eq. (17) for g_{ij}^{s}] is

$$g_{ij}(x)=\sum_{p=0}^{\infty}(-8x^2)^p\left[(3/2)_p+p!(2\pi)^{1/2}\xi+\sum_{k=0}^{\infty}\frac{2^{k/2+1}}{k!}\Gamma\left(\frac{k}{2}+1\right)\zeta(k+2)\left(\frac{1-k}{2}\right)_p\xi^{k+2}\right]\times\sum_{q=0}^{\infty}C(p,q)(-2\xi x)^q. \tag{26}$$

D. Small separation behavior

The behavior near $x=0$ of the pair distribution and of the corresponding pseudopotential is deduced from the last equations. It reads

$$g_{ij}(x)=g_{ij}(0)\left(1-2\xi x+2\xi^2x^2+\frac{2}{3}\xi x^3-\frac{10}{9}\xi^3x^3\right)-\frac{2}{9}\xi^2x^3\frac{d}{d\xi}[g_{ij}(0)]+O(x^4) \tag{27}$$

and

$$\frac{\lambda_{ij}}{Z_i Z_j e^2} V_{ij}(x) = \frac{1}{\xi} \ln[g_{ij}(x)] = A_{ij}\left(1 - \frac{2}{9}\xi x^3\right) - 2x + \frac{2}{3}x^3 + \frac{2}{9}\xi^2 x^3 - \frac{2}{9}\xi^2 x^3 \frac{dA_{ij}}{d\xi} + O(x^4), \tag{28}$$

with

$$A_{ij} = \frac{\lambda_{ij}}{Z_i Z_j e^2} V_{ij}(0) = \frac{1}{\xi} \ln[g_{ij}(0)] = (2\pi)^{1/2} + \pi\left(\frac{\pi}{3} - 1\right)\xi + O(\xi^2). \tag{29}$$

We verify that, for $x=0$, the slope of $(\lambda_{ij}/Z_i Z_j e^2)V_{ij}(x)$ is -2,

$$\left[\frac{d}{dx}\left(\frac{\lambda_{ij}}{Z_i Z_j e^2} V_{ij}(x)\right)\right]_{x=0} = -2. \tag{30}$$

This is a known result [23]. Figure 1 in Ref. [2] shows A_{ij} as a function of ξ^2 for $\epsilon = +1$ and -1 [Eq. (9)].

In the case of small distance, an approximation to g_{ij} is

$$g_{ij}(x) = g_{ij}(0)\exp(-2\xi x) \quad \text{for small } |\xi x|. \tag{31}$$

Here, "small distance" means $r < \lambda/\xi$.

E. High temperature limit

The high temperature limit is the small $|\xi|$ limit. Starting from expansion (26) and taking account of Eq. (12), we arrive at

$$g_{ij}(x) = 1 + (2\pi)^{1/2}\xi - 4\xi x \sum_{p=0}^{\infty} \frac{(3/2)_p(-8x^2)^p}{(2p+2)!(2p+1)} + \frac{\pi^2}{3}\xi^2 - 4(2\pi)^{1/2}\xi^2 x \sum_{p=0}^{\infty} \frac{p!(-8x^2)^p}{(2p+2)!(2p+1)} + 8\xi^2 x^2 \sum_{p=0}^{\infty} \frac{(3/2)_p(-8x^2)^p}{(2p+3)!(2p+2)} \sum_{q=1}^{2p+1} \frac{1}{q} - 4\xi^2 x^2 \sum_{p=0}^{\infty} \frac{(3/2)_p(-8x^2)^p}{2p+3} \times \sum_{q=1}^{2p+1} \frac{(-1)^q}{q!q(2p+2-q)!(2p+2-q)} + O(|\xi|^3). \tag{32}$$

In the last equation, it can be verified that the first summation over p can be expressed in terms of $\exp(-2x^2)$ and of the error function $\Phi(2^{1/2}x)$. Then, this equation is rewritten as follows:

$$g_{ij}(x) = 1 + \frac{\xi}{x}[1 - \exp(-2x^2)] + (2\pi)^{1/2}\xi[1 - \Phi(2^{1/2}x)] + \frac{\pi^2}{3}\xi^2 - 2(2\pi)^{1/2}\xi^2 x \times \sum_{p=0}^{\infty} \frac{(-4x^2)^p}{(2p+1)!!(p+1)(2p+1)} + 2\xi^2 x^2 \sum_{p=0}^{\infty} \frac{(-2x^2)^p}{(p+1)!(2p+3)} \sum_{q=1}^{2p+1} \frac{1}{q} \times \left(\frac{1}{p+1} - \frac{(-2p-2)_q}{q!(2p+2-q)}\right) + O(|\xi|^3). \tag{33}$$

Thus, in the high temperature limit, the pseudopotential is

$$\frac{\lambda_{ij}}{Z_i Z_j e^2} V_{ij}(x) = \frac{1}{x}[1 - \exp(-2x^2)] + (2\pi)^{1/2} \times [1 - \Phi(2^{1/2}x)] + O(|\xi|) \tag{34}$$

or

$$V_{ij}(r) = \frac{Z_i Z_j e^2}{r}\left[1 - \exp\left(-\frac{2r^2}{\lambda_{ij}^2}\right)\right] + \frac{Z_i Z_j e^2}{\lambda_{ij}}(2\pi)^{1/2} \times \left[1 - \Phi\left(\frac{2^{1/2} r}{\lambda_{ij}}\right)\right] + O(e^4), \tag{35}$$

which is exactly the potential derived by Kelbg and his coworkers [3,11]. It is easy to write the term of the order of ξ (or the squared interaction e^4) and the following ones correcting this potential. We proposed [17] an approximate expression for $V_{ij}(r)$. This is the Kelbg potential, which is modified in such a way that the value at origin, $(2\pi)^{1/2} Z_i Z_j e^2/\lambda_{ij}$, is replaced with the exact one: $A_{ij} Z_i Z_j e^2/\lambda_{ij}$ where A_{ij} is defined by Eq. (29). This approximate expression is

$$V_{ij}(r) \simeq \frac{Z_i Z_j e^2}{r}\left[1 - \exp\left(-\frac{2r^2}{\lambda_{ij}^2}\right)\right] + \frac{Z_i Z_j e^2}{\lambda_{ij}} A_{ij} \times \left[1 - \Phi\left(\frac{2(\pi)^{1/2} r}{A_{ij}\lambda_{ij}}\right)\right]. \tag{36}$$

It reproduces exactly the value at the origin, the slope at the origin, and as expected there is no term in r^2 in the r expansion. Recently, Wagenknecht and co-workers have proposed exactly the same approximation [24].

Rahal proposed another generalization of Eq. (36) in order to represent the interaction between an electron and a hydrogenlike ion. Doing that, he took account of the ion extension [25].

F. Low temperature limit

To study the low temperature limit (i.e., the high $|\xi|$ limit), the results due to Davies and Storer [4] are used and generalized when x does not equal 0. The two cases $\epsilon = +1$ and $\epsilon = -1$ are considered separately.

1. Case of like charge signs

In this case ξ is negative. Davies and Storer estimated $g_{ij}(0)$ by the steepest descent method and wrote it in the form

$$g_{ij}(0) \approx \frac{2}{3^{1/2}}(-2\pi\xi)^{4/3}\exp\left(-3\frac{(-\pi\xi)^{2/3}}{2^{1/3}}\right) \quad \text{for large } |\xi|, \tag{37}$$

which gives

$$\begin{aligned}\xi^3\left(\frac{1}{\xi}\frac{d}{d\xi}\right)^p \xi^{-3} g_{ij}(0) &\approx \frac{(-1)^p 2^{(2p+7)/3}\pi^{2(p+2)/3}}{3^{1/2}(-\xi)^{4(p-1)/3}} \\ &\quad \times \exp\left(-3\frac{(-\pi\xi)^{2/3}}{2^{1/3}}\right) \quad \text{for large } |\xi|.\end{aligned} \tag{38}$$

In the last equation, only the main term (in the large $|\xi|$ limit) is kept. Starting from Eq. (24), it is possible to write

$$\begin{aligned} g_{ij}(x) &\approx \frac{2}{3^{1/2}}(-2\pi\xi)^{4/3}\exp\left(-3\frac{(-\pi\xi)^{2/3}}{2^{1/3}}\right)\sum_{p=0}^{\infty}(-1)^p \\ &\quad \times [2(-2\pi\xi)^{1/3}x]^{2p}\sum_{q=0}^{\infty} C(p,q) \\ &\quad \times (-2\xi x)^q \quad \text{for large } |\xi|. \end{aligned} \tag{39}$$

This equation can be rewritten in terms of increasing powers of x. For each power of x, the main term (for large $|\xi|$) corresponds to $p=0$. Therefore, taking into account only $p=0$ and expressing $C(0,q)$ [Eq. (13)], Eq. (39) becomes

$$\begin{aligned} g_{ij}(x) &\approx g_{ij}(0)\sum_{q=0}^{\infty} C(0,q)(-2\xi x)^q \\ &\approx \frac{2}{3^{1/2}}(-2\pi\xi)^{4/3}\exp\left(-3\frac{(-\pi\xi)^{2/3}}{2^{1/3}}\right) \\ &\quad \times \sum_{q=0}^{\infty}\frac{(2q)!(-2\xi x)^q}{(q+1)!(q!)^3} \quad \text{for large } |\xi|. \end{aligned} \tag{40}$$

Note that the first terms in the last summation equal the first terms in the expansion of $\exp(-2\xi x)$ until order x^2. Thus we can propose, in the case of large $|\xi|$ and small $|\xi x|$, another approximation for g_{ij}:

$$g_{ij}(x) \approx \frac{2}{3^{1/2}}(-2\pi\xi)^{4/3}\exp\left(-3\frac{(-\pi\xi)^{2/3}}{2^{1/3}} - 2\xi x\right) \quad \text{for large } |\xi| \text{ and small } |\xi x|. \tag{41}$$

2. Case of unlike charge signs

In this case, as noted by Davies and Storer, the bound states dominate for large ξ (which is positive). Thus Eq. (20) yields

$$g_{ij}(x) \approx 2(2\pi)^{1/2}\xi^3\exp\left(\frac{\xi^2}{2} - 2\xi x\right) \quad \text{for large } \xi \text{ and small } \xi x. \tag{42}$$

All the last approximations [Eqs. (40)–(42)] have good behaviors for small x: the expansions of $[\lambda_{ij}/(Z_iZ_je^2)]V_{ij}(x)(=\ln[g_{ij}(x)]/\xi)$ in increasing powers of x are the good ones until the second order.

Note that the approximations (41) and (42) are valid only in the case where the separation distance is small (see the end of Sec. II D).

III. PAIR OF ELECTRONS

A. Expansion of g_{ee}

In the case of a pair of electrons, the wave functions have to be antisymmetric. Thus, if the pair of electrons is in a triplet state, the wave function is antisymmetric for the exchange of the positions, and if the pair of electrons is in a singlet state, the wave function is symmetric for the exchange of the positions. Let g_{ee}^T and g_{ee}^S be the pair distribution functions for two electrons in a triplet state and in a singlet state, respectively. For g_{ee}^T, Eq. (7) is modified as

$$\begin{aligned} g_{ee}^T(r) &= \frac{\rho_2(\mathbf{x},\mathbf{y},\mathbf{x},\mathbf{y},\beta) - \rho_2(\mathbf{x},\mathbf{y},\mathbf{y},\mathbf{x},\beta)}{\rho_1(\mathbf{x},\mathbf{x},\beta)\rho_1(\mathbf{y},\mathbf{y},\beta)} \\ &= \left(\frac{\pi}{2}\right)^{1/2}\lambda_{ij}^3\int_0^\infty dk\, k^2\alpha\frac{\exp\left(-\frac{1}{2}\lambda_{ij}^2k^2\right)}{\exp(2\pi\alpha)-1}\int_{-1}^{+1}du \\ &\quad \times [e^{ikru}\,{}_1F_1(-i\alpha,1;ik(r-ru)) \\ &\quad - e^{-ikru}\,{}_1F_1(-i\alpha,1;ik(r+ru))] \\ &\quad \times [e^{-ikru}\,{}_1F_1(i\alpha,1;-ik(r-ru)) \\ &\quad - e^{ikru}\,{}_1F_1(i\alpha,1;-ik(r+ru))] \\ &= -8(2\pi)^{1/2}\xi^3\int_0^\infty dK\, K\frac{\exp(-2\xi^2K^2)}{\exp(\pi/K)-1}(A-B), \end{aligned} \tag{43}$$

with

$$B=\frac{1}{2}\int_{-1}^{+1}du\,{}_1F_1\left(1+\frac{\mathrm{i}}{2K},1;2\mathrm{i}\xi Kx(1-u)\right)\times{}_1F_1\left(1-\frac{\mathrm{i}}{2K},1;-2\mathrm{i}\xi Kx(1+u)\right), \tag{44}$$

$$K=\frac{k\hbar^2}{e^2m_e}=k\lambda\!\!\!^{-}_{ee}/2|\xi|,\quad \text{and}\quad x=r/\lambda\!\!\!^{-}_{ee}, \tag{45}$$

where m_e is the electron mass. In a similar manner, g_{ee}^S reads

$$g_{ee}^S(r)=\frac{\rho_2(\mathbf{x},\mathbf{y},\mathbf{x},\mathbf{y},\beta)+\rho_2(\mathbf{x},\mathbf{y},\mathbf{y},\mathbf{x},\beta)}{\rho_1(\mathbf{x},\mathbf{x},\beta)\rho_1(\mathbf{y},\mathbf{y},\beta)}=-8(2\pi)^{1/2}\xi^3\int_0^\infty dK\,K\frac{\exp(-2\xi^2K^2)}{\exp(\pi/K)-1}(A+B). \tag{46}$$

Therefore, we get the relation

$$g_{ee}(x)=\frac{3}{4}g_{ee}^T(r)+\frac{1}{4}g_{ee}^S(r)=-8(2\pi)^{1/2}\xi^3\int_0^\infty dK\,K\frac{\exp(-2\xi^2K^2)}{\exp(\pi/K)-1}\left(A-\frac{1}{2}B\right). \tag{47}$$

A is expressed in the preceding section [Eq. (11)]. B has also been expanded in increasing powers of K^2:

$$B=\sum_{p=0}^{\infty}(-1)^p(4\xi Kx)^{2p}\sum_{q=0}^{\infty}D(p,q)(-2\xi x)^q, \tag{48}$$

with

$$D(p,q)=\frac{1}{(2p+q+1)!}\sum_{n=0}^{2p}(-1)^n\times\sum_{m=0}^{q}\frac{\mathcal{S}_{m+n+1}^{(m+1)}\mathcal{S}_{q-m+2p-n+1}^{(q-m+1)}}{(m+n)!(q-m+2p-n)!}. \tag{49}$$

In Eq. (47), the integration over K is evaluated exactly as done in the case of distinguishable particles. Then, g_{ee} becomes

$$g_{ee}(x)=\xi^3\sum_{p=0}^{\infty}\left[\left(\frac{1}{\xi}\frac{d}{d\xi}\right)^p[2\xi^{-3}g_{ee}(0)]\right]\times\sum_{q=0}^{\infty}\left[C(p,q)-\frac{1}{2}D(p,q)\right](-2\xi x)^{2p+q}. \tag{50}$$

Note that $g_{ee}(0)$ is half the value of $g_{ee}^{no\ exc}(0)$, the pair distribution function at the origin, in the case where the exchange is not taken into account [4]. Thus, $2g_{ee}(0)$ is expressed by Eq. (25). The expansion of g_{ee} in increasing powers of x and ξ [analogous with Eq. (26)] reads

$$g_{ee}(x)=\sum_{p=0}^{\infty}(-8x^2)^p\left[\left(\frac{3}{2}\right)_p+p!(2\pi)^{1/2}\xi+\sum_{k=0}^{\infty}\frac{2^{k/2+1}}{k!}\times\Gamma\left(\frac{k}{2}+1\right)\zeta(k+2)\left(\frac{1-k}{2}\right)_p\xi^{k+2}\right]\times\sum_{q=0}^{\infty}\left[C(p,q)-\frac{1}{2}D(p,q)\right](-2\xi x)^q. \tag{51}$$

Compare $C(p,q)$ [Eq. (12)] with the term $[C(p,q)-\frac{1}{2}D(p,q)]$, which is

$$C(p,q)-\frac{1}{2}D(p,q)=\frac{1}{(2p+q+1)!}\sum_{n=0}^{2p}(-1)^n\times\sum_{m=0}^{q}\frac{\mathcal{S}_{m+n+1}^{(m+1)}\mathcal{S}_{q-m+2p-n+1}^{(q-m+1)}}{(m+n)!(q-m+2p-n)!}\times\left[\frac{(2p+q)!}{(m+n)!(q-m+2p-n)!}-\frac{1}{2}\right]. \tag{52}$$

They differ by the term $-\frac{1}{2}$ in the factor $[(2p+q)!/(m+n)!(q-m+2p-n)!-\frac{1}{2}]$. This is due to the exchange within the pair of electrons.

B. Small separation behavior

From Eq. (50), the behaviors of g_{ee} and V_{ee} near $x=0$ can be deduced. Thus,

$$g_{ee}(x)=g_{ee}(0)\left(1-2\xi x+2x^2+\frac{8}{3}\xi^2x^2-\frac{4}{3}\xi x^3-\frac{16}{9}\xi^3x^3\right)-\frac{2}{3}\left(\xi x^2-\frac{2}{3}\xi^2x^3\right)\frac{d}{d\xi}g_{ee}(0)+O(x^4) \tag{53}$$

and

$$\begin{aligned}\frac{\lambda_{ee}}{e^2}V_{ee}(x)&=\frac{1}{\xi}\ln[g_{ee}(x)]=-\frac{\ln(2)}{\xi}+\frac{\lambda_{ee}}{e^2}V_{ee}^{no\ exc}(0)\\&\quad-2x+\frac{2}{\xi}x^2+\frac{2}{3}\xi x^2+\frac{8}{3}x^3+\frac{8}{9}\xi^2x^3\\&\quad-\frac{2}{3}\left(x^2-\frac{2}{3}\xi x^3\right)\frac{d}{d\xi}\ln[2g_{ee}(0)]+O(x^4)\\&=-\frac{\ln(2)}{\xi}+A_{ee}\left(1-\frac{2}{3}x^2+\frac{4}{9}\xi x^3\right)\\&\quad-2x+\frac{2}{\xi}x^2+\frac{2}{3}\xi x^2+\frac{8}{3}x^3+\frac{8}{9}\xi^2x^3\\&\quad-\frac{2}{3}\left(\xi x^2-\frac{2}{3}\xi^2x^3\right)\frac{dA_{ee}}{d\xi}+O(x^4).\end{aligned}\tag{54}$$

A_{ee} is defined as is done in the case of distinguishable particles [see Eq. (29)], i.e.,

$$\begin{aligned}A_{ee}&=\frac{\lambda_{ee}}{e^2}V_{ee}^{no\ exc}(0)=\frac{1}{\xi}\ln[g_{ee}^{no\ exc}(0)]\\&=\frac{1}{\xi}\ln[2g_{ee}(0)]=(2\pi)^{1/2}+\pi\left(\frac{\pi}{3}-1\right)\xi+O(\xi^2),\end{aligned}\tag{55}$$

where $V_{ee}^{no\ exc}(0)$ is the pseudopotential at the origin if the exchange between the two electrons is neglected. Equation (54) can be rewritten as follows:

$$V_{ee}(r)=k_BT\ln(2)+V_{ee}^{no\ exc}(0)-\frac{2e^2r}{\lambda_{ee}^2}+O(r^2).\tag{56}$$

Looking at the last equation, we remark that $k_BT\ln(2)$ is a purely exchange term. In the expansion of $V_{ee}(r)$ with respect to r, there is a term of the order of r^2, in contrast to the unlike particle case. Note that the slope at the origin has the same value as in the case of unlike particles. We have compared Eq. (53) with the results of Isihara and Wadati [26] [see Eq. (2.13) in their paper]. We do not completely agree with them.

C. High temperature limit

In this limit, $g_{ee}(x)$ expressed by Eq. (51), is expanded with respect to ξ:

$$\begin{aligned}g_{ee}(x)&=\frac{1}{2}[1+(2\pi)^{1/2}\xi-2\xi x]\\&\quad+\sum_{p=1}^{\infty}(-8x^2)^p[(3/2)_p+p!(2\pi)^{1/2}\xi]\\&\quad\times\left\{-\frac{1}{2(2p+1)!}-2\xi x\left[C(p,1)-\frac{1}{2}D(p,1)\right]\right\}\\&\quad+O(\xi^2),\end{aligned}\tag{57}$$

with

$$C(p,1)-\frac{1}{2}D(p,1)=\frac{1}{(2p+2)!}\left(\frac{1}{2p+1}-\sum_{q=0}^{p-1}\frac{1}{2q+1}\right).\tag{58}$$

This expansion is then rewritten as

$$\begin{aligned}g_{ee}(x)&=1+(2\pi)^{1/2}\xi-\frac{1}{2}\sum_{p=0}^{\infty}\frac{(3/2)_p(-8x^2)^p}{(2p+1)!}\\&\quad-4\xi x\sum_{p=0}^{\infty}\frac{(3/2)_p(-8x^2)^p}{(2p+2)!(2p+1)}\\&\quad-\left(\frac{\pi}{2}\right)^{1/2}\xi\sum_{p=0}^{\infty}\frac{p!(-8x^2)^p}{(2p+1)!}\\&\quad+2\xi x\sum_{p=0}^{\infty}\frac{(3/2)_p(-8x^2)^p}{(2p+2)!}\sum_{q=0}^{p}\frac{1}{2q+1}+O(\xi^2)\\&=1-\frac{1}{2}\exp(-2x^2)+\frac{\xi}{x}[1-\exp(-2x^2)]\\&\quad+(2\pi)^{1/2}\xi[1-\Phi(2^{1/2}x)]-(2\pi)^{1/2}\xi G(x)+O(\xi^2),\end{aligned}\tag{59}$$

where

$$\begin{aligned}G(x)&=\frac{1}{2}{}_1F_1\left(1,\frac{3}{2};2x^2\right)+\frac{1}{2(2\pi)^{1/2}x}\\&\quad\times\sum_{p=1}^{\infty}\frac{(-2x^2)^p}{p!}\sum_{q=0}^{p-1}\frac{1}{2q+1}\\&=\frac{1}{2}\exp(-2x^2)\left[{}_1F_1\left(\frac{1}{2},\frac{3}{2};2x^2\right)\right.\\&\quad\left.-\frac{2^{1/2}x}{\pi^{1/2}}{}_2F_2\left(1,1,\frac{3}{2},2,2x^2\right)\right]\end{aligned}\tag{60}$$

$$=\frac{1}{2}\exp(-2x^2)\sum_{n=0}^{\infty}\frac{(-2^{1/2}x)^n}{(n+1)\Gamma\left(\frac{n}{2}+1\right)}.\tag{61}$$

In Eq. (59), the Gaussian term $\frac{1}{2}\exp(-2x^2)$, corresponds to the case of the ideal Fermi gas (exchange without interaction), the two following terms are Kelbg's potential (interaction without exchange), and $(2\pi)^{1/2}\xi G(x)$ is an exchange term (with interaction). $G(x)$ decreases quickly as x increases. Equations (57) and (60) are in agreement with Matsuda's results [27]. It can be verified that ν_q^{ex} evaluated by Trubnikov and Elesin [8] [see Eq. (1.15) in their paper] is exactly

$$\nu_q^{ex}(x) = -\tfrac{1}{2}\exp(-2x^2) - (2\pi)^{1/2}\xi G(x), \tag{62}$$

in agreement with us. The pseudopotential to Eq. (59) is

$$\begin{aligned}\frac{\lambda_{ee}}{e^2}V_{ee}(x) = \frac{1}{\xi}\ln[g_{ee}(x)] = \frac{1}{\xi}\ln\left[1-\frac{1}{2}\exp(-2x^2)\right] \\ + \left[1-\frac{1}{2}\exp(-2x^2)\right]^{-1} \\ \times\left\{\frac{1}{x}[1-\exp(-2x^2)] + (2\pi)^{1/2}\right. \\ \left.\times[1-\Phi(2^{1/2}x) - G(x)]\right\} + O(|\xi|)\end{aligned} \tag{63}$$

or

$$\begin{aligned}V_{ee}(r) = -k_BT\ln\left[1-\frac{1}{2}\exp\left(-\frac{2r^2}{\lambda_{ee}^2}\right)\right] \\ + \left[1-\frac{1}{2}\exp\left(-\frac{2r^2}{\lambda_{ee}^2}\right)\right]^{-1} \\ \times\left\{\frac{e^2}{r}\left[1-\exp\left(-\frac{2r^2}{\lambda_{ee}^2}\right)\right] + \frac{e^2}{\lambda_{ee}}(2\pi)^{1/2}\right. \\ \left.\times\left[1-\Phi\left(\frac{2^{1/2}r}{\lambda_{ee}}\right) - G\left(\frac{r}{\lambda_{ee}}\right)\right]\right\} + O(e^4).\end{aligned} \tag{64}$$

As we have done in the case of distinguishable particles, we propose an approximate expression for $V_{ee}(r)$:

$$\begin{aligned}V_{ee}(r) \simeq -k_BT\ln\left[1-\frac{1}{2}\exp\left(-\frac{2r^2}{\lambda_{ee}^2}\right)\right] \\ + \left[1-\frac{1}{2}\exp\left(-\frac{2r^2}{\lambda_{ee}^2}\right)\right]^{-1}\left\{\frac{e^2}{r}\left[1-\exp\left(-\frac{2r^2}{\lambda_{ee}^2}\right)\right]\right. \\ + \frac{e^2}{\lambda_{ee}}A_{ee}\left[1-\Phi\left(\frac{2(\pi)^{1/2}}{A_{ee}}\frac{r}{\lambda_{ee}}\right)\right. \\ \left.\left.-G\left(\frac{(2\pi)^{1/2}}{A_{ee}}\frac{r}{\lambda_{ee}}\right)\right]\right\}.\end{aligned} \tag{65}$$

The last expression reproduces the good value at the origin, the good slope at the origin, and its large r behavior is e^2/r, the Coulomb potential.

D. Low temperature limit

For this limit, we process exactly as in the case of distinguishable particles. Using the relation (38) and expressing $C(0,q) - \frac{1}{2}D(0,q)$, Eq. (50) becomes

$$\begin{aligned}g_{ee}(x) \approx \frac{2(-2\pi\xi)^{4/3}}{3^{1/2}}\exp\left(-3\frac{(-\pi\xi)^{2/3}}{2^{1/3}}\right) \\ \times\sum_{q=0}^{\infty}\frac{(-2\xi x)^q}{(q+1)!q!} \\ \times\left[\frac{(2q)!}{(q!)^2} - 2^{q-1}\right] \quad \text{for large } |\xi|.\end{aligned} \tag{66}$$

As is done for unlike particles, we propose another approximation:

$$\begin{aligned}g_{ee}(x) \approx \frac{(-2\pi\xi)^{4/3}}{3^{1/2}}\exp\left(-3\frac{(-\pi\xi)^{2/3}}{2^{1/3}} - 2\xi x\right) \\ \text{for large } |\xi| \quad \text{and small } |\xi x|.\end{aligned} \tag{67}$$

The last approximation is half of approximation (41), which is in agreement with the small x behavior.

IV. CONCLUSION

Pair distribution functions [Eqs. (1) and (2)] and the corresponding pseudopotentials have been studied. The expansions with respect to x and ξ are exactly derived. Some expressions are proposed in order to approach the pseudopotentials. They fit the known limits. These expressions are made to be used in the framework of classical statistical mechanics instead of the Coulomb potential. This is valid for low enough densities. In order to neglect the case where three particles are near, the mean interparticle distance has to be larger than the de Broglie length.

In the case of high temperature, the approximations (36) and (65) are more accurate than those proposed by us earlier [Eqs. (5.10) or (5.19) in Ref. [1]] and already used to study plasma properties [12–20]. For infinite temperature ($|\xi| \to 0$), Eq. (36) yields the Kelbg potential [3], which is an exact result. The simple approximate expressions proposed in Ref. [1] can be used easily and permit some calculations without any computer. This way, quantum corrections to classical properties of plasmas can be simply studied. But for accurate comparisons with exact quantum results, the approximations proposed here are better.

[1] H. Minoo, M.-M. Gombert, and C. Deutsch, Phys. Rev. A **23**, 924 (1981).
[2] M.-M. Gombert, H. Minoo, and C. Deutsch, Phys. Rev. A **29**, 940 (1984).
[3] G. Kelbg, Ann. Phys. (Leipzig) **12**, 219 (1963); **12**, 314 (1964).
[4] B. Davies and R.G. Storer, Phys. Rev. **171**, 150 (1968). We remark that there is a little mistake: the contribution of bound states has to be divided by 4π. Thus the results are the right ones for like particles but not for unlike particles. Equation (10) in this paper can be generalized to get our Eq. (25). The quantum parameter used by these authors was $\gamma=2\xi^2$.
[5] K. Rohde, G. Kelbg, and W. Ebeling, Ann. Phys. (Leipzig) **22**, 1 (1968).
[6] R.G. Storer, J. Math. Phys. **9**, 964 (1968).
[7] A. Barker, Aust. J. Phys. **21**, 121 (1968); Phys. Rev. **179**, 129 (1969); J. Chem. Phys. **55**, 1751 (1971).
[8] B.A. Trubnikov and V.F. Elesin, Zh. Eksp. Teor. Fiz. **47**, 1279 (1964) [Sov. Phys. JETP **20**, 866 (1965)].
[9] P. Vieillefosse, J. Stat. Phys. **74**, 1195 (1994); **80**, 461 (1995).
[10] G. Kelbg and H. Hetzheim, Ann. Phys. (Leipzig) **20**, 68 (1967).
[11] W.-D. Kraeft, D. Kremp, W. Ebeling, and G. Röpke, *Quantum Statistics of Charged Particle Systems* (Plenum Press, New York, 1989).
[12] C. Deutsch and M.-M. Gombert, J. Math. Phys. **17**, 1077 (1976).
[13] C. Deutsch, Ann. Phys. (N.Y.) **115**, 404 (1978); Phys. Rev. A **17**, 909 (1978).
[14] C. Deutsch, M.-M. Gombert, and H. Minoo, Phys. Lett. A **66**, 381 (1978); **72A**, 481 (1978).
[15] C. Deutsch, Y. Furutani, and M.-M. Gombert, Phys. Rep. **69**, 85 (1981).
[16] C. Deutsch, M.-M. Gombert, and B. Held, Ann. Phys. (Paris) **17**, 465 (1982).
[17] M.-M. Gombert and H. Minoo, Contrib. Plasma Phys. **29**, 355 (1989).
[18] V. Zehnle, B. Bernu, and J. Wallenborn, Phys. Rev. A **33**, 2043 (1986); J. Phys. (Paris) **49**, 1147 (1988).
[19] R. Cauble and W. Rozmus, Phys. Fluids **28**, 3387 (1985); Phys. Lett. A **117**, 345 (1986).
[20] Yu.V. Arkhipov, F.B. Baimbetov, and A.E. Davletov, Eur. Phys. J. D **8**, 299 (2000).
[21] A. Messiah, *Mécanique Quantique* (Dunod, Paris, 1964).
[22] *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables*, edited by M. Abramowitz and I.A. Stegun (NBS, Washington, D.C., 1972).
[23] G. Pastore, G. Senatore, and M.P. Tosi, Phys. Lett. A **84**, 369 (1981).
[24] H. Wagenknecht, W. Ebeling, and A. Förster, Contrib. Plasma Phys. **41**, 15 (2001).
[25] H. Rahal, doctorat thesis, Université de Paris–Sud, 1995.
[26] A. Isihara and M. Wadati, Physica (Amsterdam) **57**, 237 (1972).
[27] K. Matsuda, Phys. Fluids **11**, 328 (1968).