Coulomb-like effective interactions for electrons with parallel spins at high temperature

M.-M. Gombert, H. Minoo, and C. Deutsch

Laboratoire de Physique des Gaz et des Plasmas, Laboratoire associé au Centre National de la Recherche Scientifique, Bâtiment 212, Université de Paris XI, F-91405 Orsay Cedex, France

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Temperature-dependent and Coulomb-like interactions taking into account short-ranged quantum effects are reviewed for nonrelativistic and hydrogenic pairs of pointlike charges of either sign in a high-temperature plasma with ions of arbitrary charge Z. A particular emphasis is given to the pseudopotential within a pair of electrons with parallel spins. Closed-form and accurate expressions are derived and compared with numerical values.

I. INTRODUCTION

The pseudopotential method is an approach to small (albeit significant) quantum corrections to the equilibrium thermodynamics in a high-temperature plasma with charges of either sign. This potential $V_{ij}(r)$ includes the quantum effects at short distances ($r \lesssim \lambda\!\!\!^{-}_{ij}$, the thermal de Broglie wavelength; i and j refer to the particle species). It turns Coulombic at larger separations ($r > \lambda\!\!\!^{-}_{ij}$) and allows for a classical treatment of canonical equilibrium quantities.[1-3]

The purpose of this work is to reiterate and detail a few more significant properties about these effective interactions. We thus supplement Ref. 1(a) (hereafter referred to as I) with a few details for hydrogenic pairs (pairs of point-like charged particles). Then, we pay special attention to the electron↑-electron↑ (parallel spin) interactions.

More generally, the evaluation of $V_{ij}(r,\theta,\varphi,T)$ for various high-Z elements of the periodic table is more tedious than for hydrogen.[4] These potentials would be useful, for instance, in the study of the plasma created during laser- or heavy-ion-beam driven fusion.[5] For this case it is essential to have an accurate knowledge of the form of $V_{ij}(r,T)$, not only for the different components of the (D-T) plasma, but also for the plasmas arising from high-Z elements. The present formalism concerns plasmas with fully stripped ions only. We take into account only the possibility of bound states between an electron and a nucleus.

II. PSEUDOPOTENTIALS

As in I, the two-body pseudopotential $V_{ij}(x,\gamma,\epsilon)$ is defined as a function of the two-body radial distribution function $g_{ij}(x,\gamma,\epsilon)$ by

$$\frac{\lambda\!\!\!^{-}_{ij}}{Z_iZ_je^2}V_{ij}(x,\gamma,\epsilon)=-\epsilon\left[\frac{2}{\gamma}\right]^{1/2}\ln[g_{ij}(x,\gamma,\epsilon)]\ , \qquad (1)$$

expressed in a dimensionless form with

$$x=r/\lambda\!\!\!^{-}_{ij},\ \gamma=2(Z_iZ_je^2/k_BT\lambda\!\!\!^{-}_{ij})^2\ ,$$
$$\epsilon=Z_iZ_j/|Z_iZ_j|\ ,$$

and $\lambda\!\!\!^{-}_{ij}=\hbar(k_BT\mu_{ij})^{-1/2}$ (μ_{ij} is the reduced mass). The function g_{ij} can be expressed in terms of the one- and two-particle density matrices using the relations

$$g_{ij}(r)=\frac{\rho_2(\vec{x}_i,\vec{y}_j,\vec{x}_i,\vec{y}_j,\beta)}{\rho_1(\vec{x}_i,\vec{x}_i,\beta)\rho_1(\vec{y}_j,\vec{y}_j,\beta)} \qquad (2)$$

for distinguishable particles, and

$$g_{e\uparrow e\uparrow}(r)=\frac{[\rho_2(\vec{x},\vec{y},\vec{x},\vec{y},\beta)-\rho_2(\vec{x},\vec{y},\vec{y},\vec{x},\beta)]}{\rho_1(\vec{x},\vec{x},\beta)\rho_1(\vec{y},\vec{y},\beta)} \qquad (3)$$

for electrons with parallel spins. The density matrices are straightforwardly expressed through the corresponding relative wave functions. At this point it should be appreciated that the plasma (collection of field particles) itself has been evacuated through a kind of thinking experiment. Nevertheless, the pair selected out is still supposed to remain in thermal equilibrium with the previous plasma. Taking into account the possibility of bound states ($Z_iZ_j<0$), g_{ij} thus reads

$$g_{ij}(x,\gamma,\epsilon)=g_s(x,\gamma,\epsilon)+\tfrac{1}{2}(1-\epsilon)g_b(x,\gamma)\ , \qquad (4)$$

a superposition of bound- and scattered-state contributions explained, respectively, by Eqs. (2.12) and (2.19) in I.

This formalism is very general. It concerns any mass and any charged particles, if it is possible to consider them points (that excludes ions with an electronic cloud). We computed $g_{ij}(r)$ and $V_{ij}(r)$ for the electron-electron, electron-proton, electron-positron, and proton-positron systems. In fact, if we introduce appropriate units for distances and energies, the numerical results are valid for any pairs of distinguishable particles. If the distances are scaled in $\lambda\!\!\!^{-}_{ij}$ and the energies in $Z_iZ_je^2/\lambda\!\!\!^{-}_{ij}$, the results depend only on the γ parameter ($\sim 1/T$) and on the ϵ ($=+1$ for like charge signs, -1 for unlike ones). This can be seen directly from the general expressions for g_{ij} [Eqs. (2.12) and (2.19) in I] and from Eq. (1). Therefore, we can give results without specifying the particle species. Our results concerning the electron-proton, electron-positron, proton-positron, and electron↑-electron↓ (antiparallel spins) systems can be used in the case of distinguishable particles for any mass and any charge.

For instance, Table IX in I can equally well represent the electron-${}^7_3$Li nucleus radial distribution function and pseudopotential at $T=9(\mu_{e\text{-Li}}/\mu_{e\text{-}p})10^6$, $9(\mu_{e\text{-Li}}/\mu_{e\text{-}p})10^7$, and $9(\mu_{e\text{-Li}}/\mu_{e\text{-}p})10^8$ K, with all the distances divided by $3(\mu_{e\text{-Li}}/\mu_{e\text{-}p})$, and all the potential energies multiplied by $9(\mu_{e\text{-Li}}/\mu_{e\text{-}p})$, $(\mu_{e\text{-Li}}/\mu_{e\text{-}p})\simeq 1)$.

Figure 3 in I can be employed for any system and is not restricted to the electron-proton and electron-positron pairs, while the high-temperature limit ($\gamma=0$) always remains Kelbg's potential:[6]

$$\frac{\lambda\!\!\!^-_{ij}}{Z_iZ_je^2}V_{ij}^K(x)=\frac{1}{x}(1-e^{-2x^2})+\sqrt{2\pi}[1-\phi(\sqrt{2}x)] \tag{5}$$

with $\phi(u)=(2/\sqrt{\pi})\int_0^u e^{-t^2}dt$.

III. $V_{ij}(0,\gamma,\epsilon)$; THE ORIGIN BEHAVIOR

A significant result is that the $(\lambda\!\!\!^-_{ij}/Z_iZ_je^2)V_{ij}(0,\gamma,\epsilon)$ calculations for distinguishable particles may be accurately extended to any γ (even $\gamma>1$) through[1(a)]

$$g_{ij}(0,\gamma,\epsilon)=1-\epsilon\sqrt{\pi\gamma}+\sum_{n=0}^{\infty}\frac{(-\epsilon)^n}{n!}\Gamma\left[\frac{n}{2}+1\right]\zeta(n+2)\gamma^{n/2+1} \tag{6}$$

which generalizes Davies and Storer's result,[7] and Eq. (1) (see Fig. 1). $\zeta(m)$ denotes the Riemann zeta function.

Finally, it is also worthwhile to point out that when spins are ignored, the relation[1(a)]

$$\frac{\partial}{\partial x}\frac{\lambda\!\!\!^-_{ij}}{Z_iZ_je^2}V_{ij}(x,\gamma,\epsilon)\,|_{x=0}=-2\ , \tag{7}$$

holds in all cases, as shown by previous authors.[8] It works also for the electron-electron interaction when an average on the spin orientation is performed.

IV. PSEUDOPOTENTIALS FOR ELECTRONS WITH PARALLEL SPINS

We already considered at length in I the electron-electron interactions. Here, we intend to disclose closed-form and quasianalytic formulas for the particular case of parallel spins. Such a situation is of a particular concern in strongly coupled plasmas, where a given spatial direction can be selected out through a steady (albeit small) magnetic field.

First, let us recall [Eq. (3.43) of I]

$$g_{e\uparrow e\uparrow}(x,\gamma)=B\left[x^2+\left[\frac{\gamma}{2}\right]^{1/2}x^3\right]+O(x^4)\qquad (x\ll 1) \tag{8}$$

with

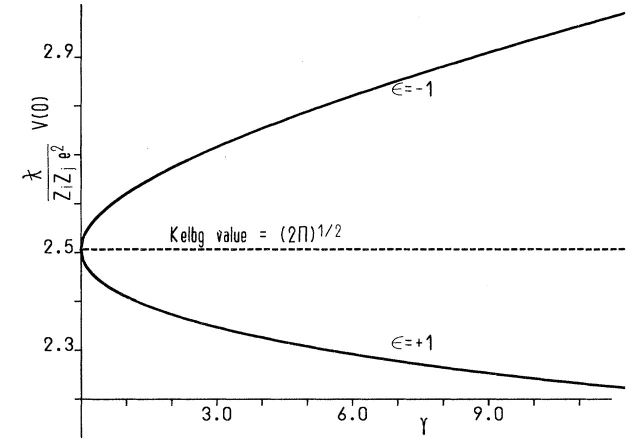

FIG. 1. $(\lambda\!\!\!^-_{ij}/Z_iZ_je^2)V_{ij}(0,\gamma)$, pseudopotential at zero separation for distinguishable particles with like and unlike charge signs.

$$B=\left[2+\frac{\gamma}{3}-\tfrac{4}{3}\gamma\frac{d}{d\gamma}\right]g_{e\uparrow e\downarrow}(0,\gamma)\ ,$$
$$B=2-\tfrac{4}{3}\sqrt{\pi\gamma}+\frac{\gamma}{3}\left[1+\frac{\pi^2}{3}\right]-\frac{\sqrt{\pi}}{3}\gamma^{3/2}+\tfrac{1}{3}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Gamma\left[\frac{n}{2}+1\right]\gamma^{n/2+1}\times[\zeta(n+2)-\zeta(n+4)]\ . \tag{9}$$

Therefore,

$$\frac{\lambda\!\!\!^-_{ee}}{e^2}V_{e\uparrow e\uparrow}(x,\gamma)=-\left[\frac{2}{\gamma}\right]^{1/2}\ln(Bx^2)-x+O(x^2)\qquad (x\ll 1)\ . \tag{10}$$

On the other hand, there is the obvious relation

$$\frac{\lambda\!\!\!^-_{ee}}{e^2}V_{e\uparrow e\uparrow}(x,\gamma)=\frac{\lambda\!\!\!^-_{ee}}{e^2}V_{e\uparrow e\downarrow}(x,\gamma)=\frac{\lambda\!\!\!^-_{ee}}{e^2}V_{ee}(x,\gamma)=\frac{1}{x}\quad (x\gg 1)\ . \tag{11}$$

The spin average

$$g_{ee}(x,\gamma)=\tfrac{1}{2}[g_{e\uparrow e\uparrow}(x,\gamma)+g_{e\uparrow e\downarrow}(x,\gamma)] \tag{12}$$

yields

$$\frac{\lambda\!\!\!^-_{ee}}{e^2}V_{e\uparrow e\uparrow}(x,\gamma)=\frac{\lambda\!\!\!^-_{ee}}{e^2}V_{e\uparrow e\downarrow}(x,\gamma)-\left[\frac{2}{\gamma}\right]^{1/2}\ln(2e^{-\sqrt{\gamma/2}h(x)}-1)\ , \tag{13}$$

where

TABLE I. Parameters C, D, E, and F used in Eqs. (16), (18), and (19) and maximum relative errors $(\Delta V/V)_{\max}$ $(=\max[\,|(\lambdabar_{ee}/e^2)V_{ee}-f\,|/(\lambdabar_{ee}/e^2)V_{ee}])$ for each case.

	T (K) 10^8	10^7	10^6
C	1.62	1.735	1.97
$\left[\frac{\Delta V}{V}\right]_{\max}(f_1)$	11%	10%	7–7.5 %
D	1.305	1.295	1.385
$\left[\frac{\Delta V}{V}\right]_{\max}(f_2)$	8–8.5 %	4–4.5 %	1.5% [$\simeq$1%, if $x>(e^2\beta/\lambdabar_{ee})$]
E	1.58	1.77	1.94
F	1.30	1.22	1.25
$\left[\frac{\Delta V}{V}\right]_{\max}(f_3)$	5.5%	4–4.5 %	5.5–6 % [$\simeq$1%, if $x>(e^2\beta/\lambdabar_{ee})$]

$$\frac{\lambdabar_{ee}}{e^2}V_{ee}(x,\gamma)=\frac{\lambdabar_{ee}}{e^2}V_{e\uparrow e\downarrow}(x,\gamma)+h(x,\gamma)\,. \tag{14}$$

In I we proposed

$$h(x,\gamma)=\left[\frac{2}{\gamma}\right]^{1/2}(\ln 2)\exp(-Cx^2/\ln 2) \tag{15}$$

with $C=2$. The corresponding approximant is

$$f_1(x,\gamma)=\frac{\lambdabar_{ee}}{e^2}V_{e\uparrow e\downarrow}(x,\gamma)-\left[\frac{2}{\gamma}\right]^{1/2}\ln[2^{1-\exp(-Cx^2/\ln 2)}-1] \tag{16}$$

with a short-range behavior

$$f_1(x,\gamma)\simeq-\left[\frac{2}{\gamma}\right]^{1/2}\ln(Cx^2)+\frac{\lambdabar_{ee}}{e^2}V_{e\uparrow e\downarrow}(0,\gamma)-2x+O(x^2)\,. \tag{17}$$

Near $x=0$, we can approach much closer the numerical values by taking $C=B/g_{e\uparrow e\downarrow}(0)$. In fact, for all distances, $C=2$ [the high-temperature limit of $B/g_{e\uparrow e\downarrow}0$] is a more convenient choice; however, the best is to determine C empirically. The C data are given in Table I.

We also propose two other formulas:

$$f_2(x,\gamma)=\frac{\lambdabar_{ee}}{e^2}V_{e\uparrow e\downarrow}(x,\gamma)-\left[\frac{2}{\gamma}\right]^{1/2}\mathrm{Ei}(-Dx^2) \tag{18}$$

TABLE II. Coefficients B_{nk} of Eq. (3.55) in I.

n	B_{n0}	B_{n1}	B_{n2}	B_{n3}	B_{n4}
2	2	$\frac{2\sqrt{\pi}}{3}$	$\frac{1}{3}\left[1+2\pi-\frac{2\pi^2}{3}\right]$	$\sqrt{\pi}\left[\zeta(3)-\frac{\pi^2}{3}+\frac{2\pi}{3}\right]$	$\frac{\pi}{3}\left[4\zeta(3)+\frac{\pi^3}{15}-\frac{4}{3}\pi^2+2\pi\right]$
3			$b_3=-\frac{2}{3}(2\gamma)^{1/2}b_2$		
4	-4	$-\frac{34\sqrt{\pi}}{15}$	$-\frac{1}{3}(\frac{1}{2}+\frac{112}{15}\pi-\frac{32}{15}\pi^2)$	$-\sqrt{\pi}[\frac{1}{18}+\frac{122}{45}\pi-\frac{167}{135}\pi^2+3\zeta(3)]$	$\frac{11}{180}-\frac{\pi}{18}-\frac{787}{270}\pi^2+\frac{248}{135}\pi^3-\frac{206}{2025}\pi^4-\frac{24}{5}\pi\zeta(3)$
5	$\frac{176\sqrt{2}}{45}$	$\frac{1592\sqrt{2\pi}}{675}$	$\frac{\sqrt{2}}{45}(41+\frac{1792}{15}\pi-\frac{512}{15}\pi^2)$	$\frac{\sqrt{2\pi}}{45}[\frac{41}{3}+148\zeta(3)-\frac{2732}{45}\pi^2+\frac{664}{5}\pi]$	$\frac{\sqrt{2}}{135}[\frac{77}{10}+\pi\zeta(3)\frac{3616}{5}+41\pi+\frac{6371}{15}\pi^2-\frac{1376}{5}\pi^3+\pi^4\frac{3416}{225}]$

with $\mathrm{Ei}(-u) = -\int_u^\infty (e^{-t}/t)dt$ $(u>0)$, and

$$f_3(x,\gamma) = \frac{\lambdabar_{ee}}{e^2} V_{e\uparrow e\uparrow}(x,\gamma) - \left[\frac{2}{\gamma}\right]^{1/2} \ln\left[\frac{Ex^2}{1+Ex^2}\right] \exp(-Fx^2) \ . \qquad (19)$$

The parameters D,E,F are empirically evaluated and displayed in Table I where the maximum relative discrepancies $(\Delta V/V)_{\max}$ for the three approximants are also given. These three formulas (f_1,f_2,f_3) are contrasted with the exact numerical data obtained in I, in Figs. 2, 3, and 4, at $T=10^8$, 10^7, and 10^6 K, respectively. They are obtained through a very efficient approximant[1(a)] (for f_1, f_2, and f_3):

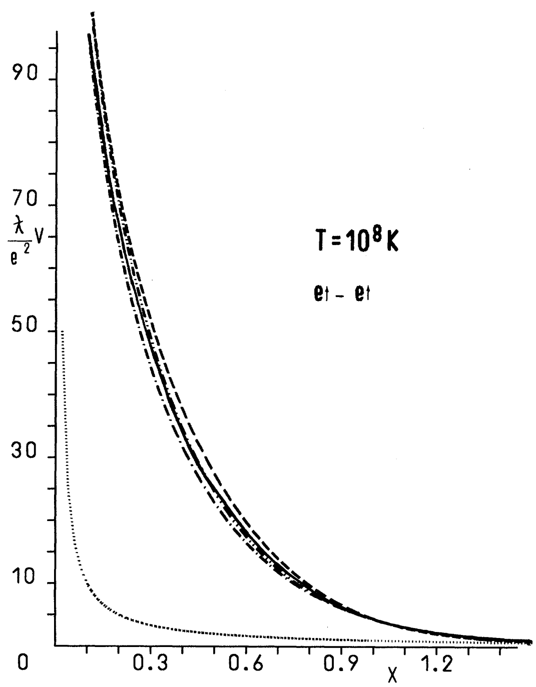

FIG. 2. Comparison between the pseudopotential $(\lambdabar_{ee}/e^2)V_{e\uparrow e\uparrow}$ (——) and its analytic approximants:

$$f_1 = (1/x)\{1-\exp[-Ax - x^2(A^2/2)-2)]\} - (2/\gamma)^{1/2}\ln[2^{1-\exp(-Cx^2/\ln 2)} - 1]$$

(– – –),

$$f_2 = (1/x)\{1-\exp[-Ax - x^2(A^2/2-2)]\} - (2/\gamma)^{1/2}\mathrm{Ei}(-Dx^2)$$

(—·—),

$$f_3 = (1/x)\{1-\exp[-Ax - x^2(A^2/2)-2)]\} - (2/\gamma)^{1/2}\ln[Ex^2/(1+Ex^2)]\exp(-Fx^2)$$

(—··—). $1/x$ is also represented (· · ·). Figure is given for $T=10^8$ K ($\gamma = 0.003\,157\,8$, $A=2.500\,76$, $C=1.62$, $D=1.305$, $E=1.58$, and $F=1.30$).

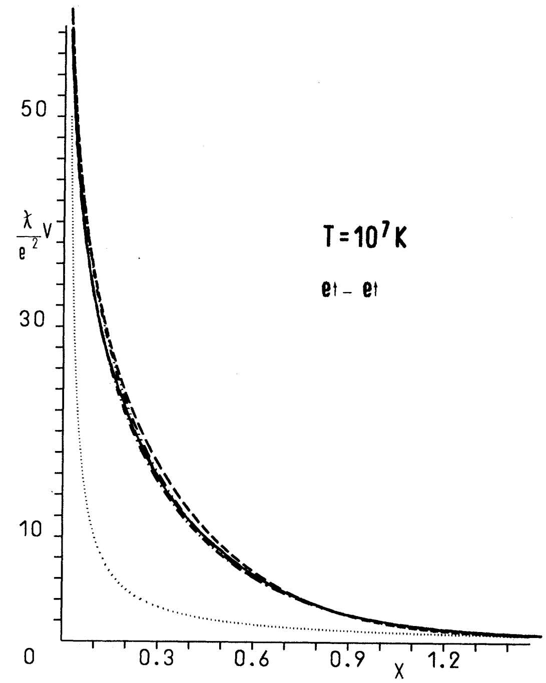

FIG. 3. Same as for Fig. 2, with $T=10^7$ K ($\gamma=0.031\,578$, $A=2.488\,25$, $C=1.735$, $D=1.295$, $E=1.77$, and $F=1.22$).

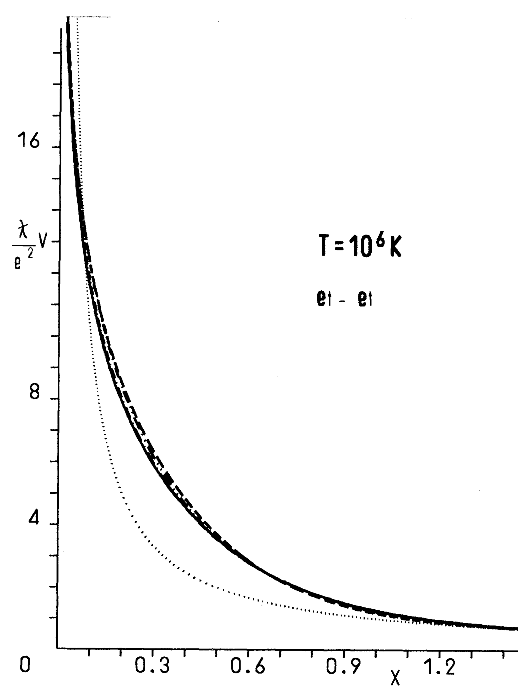

FIG. 4. Same as for Fig. 2, with $T=10^6$ K ($\gamma=0.315\,78$, $A=2.450\,22$, $C=1.97$, $D=1.385$, $E=1.94$, and $F=1.25$).

$$\frac{\lambda\!\!\!^{-}_{ee}}{e^2} V_{e\uparrow e\downarrow}(x,\gamma) \simeq \frac{1}{x}\left\{1-\exp\left[-xA - x^2\left[\frac{A^2}{2}-2\right]\right]\right\} \qquad (20)$$

with $A=(\lambda\!\!\!^{-}_{ee}/e^2)V_{e\uparrow e\downarrow}(0,\gamma)$. So, at high temperature ($T=10^8$ K) $f_3(x,\gamma)$ can be recommended while at lower temperature ($T=10^6$ K) $f_2(x,\gamma)$ is the best known approximant.

As a consequence, we expect that Eqs. (18) or (19) could provide accurate approximants for $(\lambda_{ee}/e^2)V_{e\uparrow e\uparrow}(x,\gamma)$ in various statistical physics calculations (analytical, Monte Carlo, or molecular dynamics).

Finally, in Table II we wish to supplement Table VII in I, displaying the B_{nk} coefficients [Eq. (3.55) in I] used in

$$V_{ee}(x,\gamma)=V_{ee}(0,\gamma)-k_BT\left[(2\gamma)^{1/2}x+\sum_{n=2}^{\infty} b_n x^n\right], \qquad (21)$$

where

$$b_n=\sum_{k=0}^{\infty} B_{nk}\gamma^{(\phi+k)/2}, \quad n=2,3,4,\ldots$$

and

$$\phi=\begin{cases}0 & \text{for } n \text{ even}\\ 1 & \text{for } n \text{ odd}\ .\end{cases}$$

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