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Coulomb Pair Density Matrix. II

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The Coulomb pair density matrix $G_\beta(r, r')$ for attractive and repulsive potentials and for all values of parameters is determined in the form of simple series or integrals. These results are useful in both theoretical and numerical studies.

KEY WORDS: Quantum statistical mechanics; elementary processes in plasma.

1. INTRODUCTION

In this paper, we are concerned with the density matrix $G_\beta(r, r')$ of two particles interacting through either an attractive or a repulsive Coulomb potential (like e^-p or e^-e^-). $G_\beta(r, r')$ is a function of five parameters: the two vectors r and r', the temperature β^{-1}, and the discrete variable $\varepsilon = \pm 1$, for the sign of the potential.

The normal way to study the pair density matrix is to expand it in a series of the eigenfunctions of the two-body Hamiltonian H,

$$G_\beta(r, r') = \sum_i e^{-\beta E_i} \psi_{E_i}(r)\, \psi^*_{E_i}(r')$$

This expansion involves the radial functions of the continuous spectrum of H and also the radial functions of the discrete spectrum when the potential is attractive. Thus $G_\beta(r, r')$ appears as a double series of special functions. By using this procedure, many properties have been obtained for the Coulomb pair density matrix. Of the extensive literature on that subject, we cite the following: Davies and Storer[(1)] derive the value at the origin, $G_\beta(0, 0)$; Wichmann and Woo[(2)] give a double-integral representation for

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$G_\beta(r, r')$; and Hostler[3] obtains an expression for the Laplace transform $G_\omega(r, r')$ in terms of Whittaker functions. Among the important papers concerning the effective calculation of G_β are those of Minoo *et al.*[4] and Pollock.[5] Other works on the Coulomb pair density matrix can be found in, e.g., refs. 8–10.

However, calculations starting from the series expansion over the energy eigenfunctions are rather complicated and an easier approach to $G_\beta(r, r')$ is possible. In fact, when the two-body potential $V(r)$ depends very simply on r, it appears that the density matrix is a function which is less complicated than the eigenfunctions of the Hamiltonian. A simple example of this is the case of the one-dimensional potential $V(x) = -kx$, where the eigenfunctions are Airy functions, whereas the density matrix $G_\beta(x, x')$ is simply a Gaussian.

The main reason for this simplification of G_β comes from the fact that the density matrix satisfies the two Bloch equations:

$$-\partial_\beta G_\beta(r, r') = H(r)\, G_\beta(r, r') = H(r')\, G_\beta(r, r')$$

For particular forms of $V(r)$, it follows that $G_\beta(r, r')$ has special dependences on r *and* r' or on combinations of these variables. These specific properties of course do not hold true for the eigenfunctions of the Hamiltonian; yet they represent an efficient means to calculate $G_\beta(r, r')$. In this way Hostler and Pratt[6] have shown that for the Coulomb potential, $1/r$, the density matrix depends only on two space quantities $|r| + |r'|$ and $|r - r'|$ and not on three independent quantities.

From the two Bloch equations and the property obtained by Hostler and Pratt, we derive various forms for the density matrix concerning all possible values of the five parameters with no limitation; in particular, the temperature can decrease to zero. These results allow us to calculate the density matrix simply and accurately; in most cases, a precision of 10^{-6} can be obtained with a pocket calculator.

We first introduce various notations and definitions and examine some properties of the density matrix. We then derive its expansion in power of β, the first term of which was the subject of our initial paper.[7] Next we show that the self-function $G_\beta(r, r)$ and the exchange function $G_\beta(r, -r)$ each satisfy a differential equation similar to the Bloch equations for the density matrix in the general case.

The coefficients of the powers of β in the density matrix expansion are functions of space variables each of which we determine in the form of a very simple series. This result allows us to calculate accurately the density matrix in the high-temperature domain ($\geqslant 1$ eV for two e^-).

Thus, we show that all of these coefficients can be deduced from the value at the origin $G_\beta(0, 0)$. This property is used to sum exactly the series in powers of β and we obtain the density matrix $G_\beta(r, r')$ in an integral form which generalizes the result of Davies and Storer for $G_\beta(0, 0)$. The density matrix is then expressed as a double integral or as the integral of a series. These expressions can be easily used to calculate the density matrix for all temperatures, particularly in the low-temperature range. Our numerical calculations agree well with those of Pollock.

Finally, we give some applications. The small-distance expansion, valid for all temperatures, shows that the density matrix tends, in the limit of decreasing temperature and for finite distances, to a finite limit apart from a scale factor which is temperature dependent. The large-distance expansion of the self-function is given up to the order $\hbar^6$. Some tabulated values are included to compare results from the various methods described above.

This paper gives most of the results for computing the density matrix. Extensive results, proofs, and applications will be presented elsewhere.

2. EQUATION FOR G_τ

The relative pair density matrix $G_\tau(r, r')$ is defined by

$$G_\tau(r, r') = \langle r|\, e^{-\tau H/\hbar}\, |r'\rangle \tag{1}$$

where the time τ is related to the temperature $T = \beta^{-1}$ by

$$\tau = \beta\hbar = \hbar/T \tag{2}$$

H is the two-body Hamiltonian

$$H = -\frac{\hbar^2}{2m}\Delta + V(r), \qquad V(r) = \frac{\varepsilon\alpha}{r} \quad (\varepsilon = \pm 1, \alpha > 0) \tag{3}$$

m is the reduced mass, and repulsive and attractive potentials correspond respectively to $\varepsilon = +1$ and $\varepsilon = -1$. We will also use ε as a coupling parameter when calculating expansions in powers of the potential. The distances r and r' can be expressed in units of the de Broglie thermal wavelength or in units of the Bohr radius; thus we introduce the following notations:

$$\sigma = |r - r'| = 2\mu \left(\frac{\hbar\tau}{2m}\right)^{1/2}, \qquad a = |r| + |r'| = 2\nu \left(\frac{\hbar\tau}{2m}\right)^{1/2} \quad (\mu \leqslant \nu) \tag{4}$$

$$r^* = r\,\frac{2m\alpha}{\hbar^2}, \qquad \tau^* = \tau\,\frac{2m\alpha^2}{\hbar^3}$$

$$x = \nu^2 - \mu^2, \qquad z = \nu^2, \qquad y = \mu^2 \qquad (0 \leqslant x \leqslant z)$$

$$\xi = 2\sqrt{\tau^*}\sqrt{z} = a^*, \qquad \eta = 2\sqrt{\tau^*}\sqrt{x} = (a^{*2} - \sigma^{*2})^{1/2},$$

$$\zeta = 2\sqrt{\tau^*}\sqrt{y} = \sigma^*$$

The exchange case $r' = -r$ corresponds to $\nu = \mu$ or $x = 0$ and the self-case $r' = r$ corresponds to $\mu = 0$ or $x = z$.

In the perfect gas limit $(\varepsilon \to 0)$ G_τ tends to G_τ^0,

$$G_\tau^0(r, r') = \left(\frac{m}{2\pi\hbar\tau}\right)^{3/2} e^{-\mu^2} \tag{5}$$

The effective potential $P_\tau(r, r')$ is defined by

$$G_\tau(r, r') = G_\tau^0(r, r')\, e^{-P_\tau(r,r')} = \left(\frac{m}{2\pi\hbar\tau}\right)^{3/2} \tilde{K}_\tau(r, r') \tag{6}$$

where

$$\tilde{K}_\tau(r, r') = e^{-\mu^2} K_\tau(r, r') = e^{-\mu^2 - P_\tau(r,r')} \tag{7}$$

From the definition (1) of G_τ, we derive the two Bloch equations

$$\begin{aligned} &\hbar\,\partial_\tau G_\tau(r, r') = \left\{\frac{\hbar^2}{2m}\Delta - V(r)\right\} G_\tau(r, r') = \left\{\frac{\hbar^2}{2m}\Delta' - V(r')\right\} G_\tau(r, r') \\ &G_\tau(r, r') \xrightarrow[\tau \to 0]{} \delta(r - r') \end{aligned} \tag{8}$$

G_τ is, *a priori*, a spatial function of $|r|$, $|r'|$, and θ, the angle between the two vectors r and r'. We also can use the quantities σ and a given in (4), and $b = |r| - |r'|$. From the symmetry in the exchange of r and r', it follows that G_τ has to be an even function of b. Since the Coulomb potential is weakly singular near the origin, P_τ is everywhere finite, and for $\tau \to 0$, G_τ tends to G_τ^0, which does not depend on b. Now, the special dependence of V on $r = (a + b)/2$ leads to a G_τ which does not depend on b for all values of τ. This property, which is not obvious, has been shown by Hostler and

Pratt.[6] Then G_τ depends only on the two spatial variables σ and a, and, from (8), we deduce the two differential equations

$$\frac{\partial}{\partial \tau^*}\left(\frac{\tilde{K}_\tau}{\tau^{*3/2}}\right)_{\sigma,a} = D_0^*\left(\frac{\tilde{K}_\tau}{\tau^{*3/2}}\right) \tag{9}$$

$$\frac{\partial}{\partial \tau^*}\left(\frac{\tilde{K}_\tau}{\tau^{*3/2}}\right)_{\sigma,a} = D_1^*\left(\frac{\tilde{K}_\tau}{\tau^{*3/2}}\right) \tag{10}$$

with the following definitions for D_0^* and D_1^*:

$$\begin{aligned}
D_0^* - D_1^* &= \frac{1}{\tau^*}\left(-\frac{\nu^2-\mu^2}{2\nu\mu}\frac{\partial^2}{\partial\mu\,\partial\nu} + \frac{1}{\nu}\frac{\partial}{\partial\nu} - \frac{\varepsilon\sqrt{\tau^*}}{\nu}\right)\\
&= 2\left(\frac{\partial^2}{\partial\eta^2} + \frac{1}{\eta}\frac{\partial}{\partial\eta} + \frac{2}{\xi}\frac{\partial}{\partial\xi} + \frac{\eta}{\xi}\frac{\partial^2}{\partial\xi\,\partial\eta} - \frac{\varepsilon}{\xi}\right)\\
D_1^* &= \frac{1}{4\tau^*}\left(\frac{\partial^2}{\partial\nu^2} + \frac{\partial^2}{\partial\mu^2} + \frac{2\nu}{\mu}\frac{\partial^2}{\partial\mu\,\partial\nu} + \frac{2}{\mu}\frac{\partial}{\partial\mu}\right)\\
&= \frac{\partial^2}{\partial\xi^2} - \left(\frac{\partial^2}{\partial\eta^2} + \frac{1}{\eta}\frac{\partial}{\partial\eta}\right)
\end{aligned} \tag{11}$$

The derivatives are taken with fixed τ^*. Therefore G_τ does not depend on the third variable b, because the two equations (9) and (10) are compatible. Moreover, it follows that

$$(D_0^* - D_1^*)\,\tilde{K}_\tau = 0 \tag{12}$$

which does not contain derivatives with respect to τ^*. The time τ^* and the coupling parameter ε appear in (12) by the product $\varepsilon\sqrt{\tau^*}$, and in both limits $\tau^* \to 0$ and $\varepsilon \to 0$, $\tilde{K}_\tau$ tends to $\tilde{K}^0 = \exp(-\mu^2)$.

3. ITERATIVE SOLUTION AND GENERAL PROPERTIES

In the variables μ, ν $(0 \leqslant \mu \leqslant \nu < \infty)$ Eq. (12) is a second-order differential equation of hyperbolic type. To solve it, we consider the following expansion in powers of $\varepsilon\sqrt{\tau^*}$:

$$\tilde{K}_\tau(\mu,\nu) = \sum_{n\geqslant 0} (-\varepsilon\sqrt{\tau^*})^n\, \tilde{K}^n(\mu,\nu) \tag{13}$$

From (12) it follows that

$$\left(\frac{\nu^2-\mu^2}{2\mu}\frac{\partial^2}{\partial\mu\,\partial\nu} - \frac{\partial}{\partial\nu}\right)\tilde{K}^n = \tilde{K}^{n-1} \tag{14}$$

The nonsingular solution, which tends to zero as $v \to \infty$, is

$$\tilde{K}^n(\mu, v) = \int_v^{+\infty} \frac{dv'}{v'^2 - \mu^2} \int_\mu^{v'} 2\mu' \, d\mu' \, \tilde{K}^{n-1}(\mu', v'), \qquad \tilde{K}^0(\mu, v) = e^{-\mu^2} \quad (15)$$

We deduce that the $\tilde{K}^n$ are entire functions of μ^2 and v, and then that $\tilde{K}_\tau$ is an entire function of $\varepsilon\sqrt{\tau^*}$, μ^2, and v. In particular, it follows that the value at the origin does not depend on the angle θ or the ratio v/μ.

We have integrated (15) up to the order 4. Complexity is rapidly increasing and we only give the first two orders:

$$\begin{aligned}
\tilde{K}^1(\mu, v) &= e^{-\mu^2} \frac{1}{2\mu} \operatorname{Log} \frac{v+\mu}{v-\mu} - \int_v^{+\infty} \frac{dv_1}{v_1^2 - \mu^2} e^{-v_1^2} \\
\tilde{K}^2(\mu, v) &= g(\mu) \frac{1}{4\mu} \operatorname{Log}^2 \frac{v+\mu}{v-\mu} - \int_\mu^v \frac{dv_1}{v_1^2 - \mu^2} g(v_1) \operatorname{Log} \frac{v^2 - v_1^2}{v^2 - \mu^2} \\
&\quad - \int_v^{+\infty} \frac{dv_1}{v_1^2 - \mu^2} g(v_1) \operatorname{Log} \frac{v_1 + v}{v_1 - v} \\
g(u) &\equiv \int_u^{+\infty} dt \, e^{-t^2}
\end{aligned} \quad (16)$$

The first function $\tilde{K}^1$, equal to $e^{-\mu^2} I(\mu, v)$ with the notation of ref. 7, has been studied in this paper. These functions $\tilde{K}^n$ are finite at all distances (even for $\mu = v$) and tend to zero at large distances. They satisfy a second differential equation. From (10) we deduce

$$\left[\frac{\partial^2}{\partial v^2} + \frac{\partial^2}{\partial \mu^2} + \frac{2v}{\mu} \frac{\partial^2}{\partial \mu \, \partial v} + \frac{2}{\mu} \frac{\partial}{\partial \mu} + 2 \left(\mu \frac{\partial}{\partial \mu} + v \frac{\partial}{\partial v} \right) - 2(n-3) \right] \tilde{K}^n(\mu, v) = 0 \quad (17)$$

This equation is compatible with (14) and will be very useful in the following, because it will allow us to obtain a second-order differential equation for the exchange function $\tilde{K}(v, v)$ and a third-order one for the self-function $\tilde{K}(\mu = 0, v)$.

4. EXCHANGE FUNCTION

Separation of variables is obtained for Eq. (10) when using v and $x = v^2 - \mu^2$ or $z = v^2$ and x. The function $\tilde{K}^n$ is an entire function of x and $\sqrt{z}$. We expand $\tilde{K}$ in powers of x,

$$\tilde{K}^n(x, z) = \sum_{p \geq 0} x^p \tilde{A}_p^n(z) \quad (18)$$

$p=0$ gives the exchange function, denoted by A,

$$\tilde{K}(x=0, z)=\tilde{A}_{p=0}(z)=\tilde{A}(z), \qquad \tilde{K}^n(x=0, z)=\tilde{A}^n_{p=0}(z)=\tilde{A}^n(z) \tag{19}$$

From (12) and (10), we deduce, respectively,

$$\begin{gathered}(p+1)\left[\frac{\partial}{\partial z}\tilde{A}^n_p+(p+1)\,\tilde{A}^n_{p+1}\right]=-\frac{\tilde{A}^{n-1}_p}{2\sqrt{z}}\\ \left[z\frac{\partial^2}{\partial z^2}+\left(z+\frac{1}{2}\right)\frac{\partial}{\partial z}+p-\frac{n-3}{2}\right]\tilde{A}^n_p=(p+1)^2\,\tilde{A}^n_{p+1}\end{gathered} \tag{20}$$

By eliminating $\tilde{A}^n_{p+1}$ between the two equations, we derive an equation for the p order alone:

$$\left[z\frac{\partial^2}{\partial z^2}+\left(z+p+\frac{3}{2}\right)\frac{\partial}{\partial z}+\left(p-\frac{n-3}{2}\right)\right]\tilde{A}^n_p=-\frac{\tilde{A}^{n-1}_p}{2\sqrt{z}}, \qquad \tilde{A}^0_p(z)=\frac{e^{-z}}{p!} \tag{21}$$

The function $\tilde{A}^0$ follows from $\tilde{K}^0=e^{-\mu^2}=e^{x-z}$.

For $p=0$, the solution of (21), which is regular at the origin and tends to zero at infinity, can be written in the form

$$\tilde{A}^n(z)=\frac{\sqrt{z}}{2^n n!}\int_1^{+\infty}dt\,\mathrm{Log}^n\frac{\sqrt{t}+1}{\sqrt{t}-1}\,e^{-tz}U\left(\frac{n-1}{2},\frac{3}{2},tz\right) \tag{22}$$

where U is the confluent hypergeometric function.[11] The limit $z\to 0$ gives back the values at the origin[1]

$$\begin{gathered}\tilde{A}^n(z=0)\equiv\tilde{a}^n_0, \qquad \tilde{a}^0_0=1, \qquad \tilde{a}^1_0=\sqrt{\pi},\\ \tilde{a}^n_0=\frac{\sqrt{\pi}}{2^{n-2}\Gamma((n-1)/2)}\zeta(n) \qquad (n\geqslant 2)\end{gathered} \tag{23}$$

$\zeta(n)$ is the Riemann zeta function. We shall also use expressions which contain $\tilde{a}^n_0$ for $n<0$ with the following convention:

$$\tilde{a}^n_0=0 \qquad (n<0) \tag{24}$$

5. SELF-FUNCTION

In the same way a differential equation for the self-function alone can be obtained by using variables v and μ or rather $z=v^2$ and $y=\mu^2$. The function $\tilde{K}^n$, which is an entire function of y and $\sqrt{z}$, is expanded in powers of y:

$$\tilde{K}^n(y, z) = \sum_{p \geqslant 0} y^p \tilde{B}_p^n(z) \tag{25}$$

For $p = 0$, we have the self-function, denoted by B,

$$\begin{aligned} \tilde{K}(y=0, z) &= \tilde{B}_{p=0}(z) = B(z) \\ \tilde{K}^n(y=0, z) &= \tilde{B}_{p=0}^n(z) = B^n(z) = \sum_{p \geqslant 0} z^p \tilde{A}_p^n(z) \end{aligned} \tag{26}$$

From (12) and (10), we deduce

$$\begin{aligned} (p+1)\, z \frac{\partial}{\partial z} \tilde{B}_{p+1}^n &= (p+1) \frac{\partial}{\partial z} \tilde{B}_p^n + \frac{\tilde{B}_p^{n-1}}{2\sqrt{z}} \\ \left[z \frac{\partial^2}{\partial z^2} + \left(z + \frac{1}{2} \right) \frac{\partial}{\partial z} + \left(p - \frac{n-3}{2} \right) \right] \tilde{B}_p^n & \\ + (p+1) \left(2z \frac{\partial}{\partial z} + p + \frac{3}{2} \right) \tilde{B}_{p+1}^n &= 0 \end{aligned} \tag{27}$$

which leads to the third-order equation for $\tilde{B}_p^n$

$$\begin{aligned} &\left[z \frac{\partial^2}{\partial z^2} + \left(z + \frac{3}{2} \right) \frac{\partial}{\partial z} - \frac{n-3}{2} \right] \left(z^{p+1} \frac{\partial}{\partial z} \tilde{B}_p^n \right) \\ &\quad = -z^{p+1/2} \left(\frac{\partial}{\partial z} + \frac{p+1/2}{2z} \right) \tilde{B}_p^{n-1}, \qquad \tilde{B}_p^0(z) = \frac{(-1)^p}{p!} \end{aligned} \tag{28}$$

$\tilde{B}_p^0$ is obtained from $\tilde{K}^0 = e^{-\mu^2} = e^{-y}$. This equation allows us to get directly the self-function without summing the $z^p \tilde{A}_p^n(z)$, (26).

6. SERIES

The functions $\tilde{A}_p^n$ and $\tilde{B}_p^n$, which are entire functions of $\sqrt{z}$, can be easily generated from the differential equations (21) and (28) with the "initial" conditions (23). The density matrix, and then P, can be calculated as triple sums of terms $(-\varepsilon\sqrt{\tau^*})^n\, x^p z^{q/2}$ or $(-\varepsilon\sqrt{\tau^*})^n\, y^p z^{q/2}$, which reduce to double sums in the exchange and self cases. The convergence when summing on n can be *extensively* improved by calculating first the P^n before summing on n:

$$P_\tau = \sum_{n \geqslant 1} (-1)^{n-1} (\varepsilon \sqrt{\tau^*})^n P^n$$

$$= -\text{Log}\left[1 + \sum_{n \geqslant 1} (-\varepsilon \sqrt{\tau^*})^n K^n\right], \qquad K^n = e^{\mu^2} \tilde{K}^n \tag{29}$$

$$P^1 = K^1, \qquad P^2 = K^2 - \tfrac{1}{2}(K^1)^2, \qquad P^3 = K^3 - K^1 K^2 + \tfrac{1}{3}(K^1)^3, \ldots$$

This point was mentioned by Pollock[5] and is clearly illustrated by the values at the origin, where the $\tilde{K}^n$ are given by the $\tilde{a}_0^n$, (23):

$$P^1 = \sqrt{\pi}, \qquad P^2 = \frac{\pi}{2}\left(\frac{\pi}{3} - 1\right) \simeq 0.074$$

$$P^3 = \sqrt{\pi}\left[\frac{1}{2}\zeta(3) - \frac{\pi^2}{6} + \frac{\pi}{3}\right] \simeq 0.0058 \tag{30}$$

The ratio P^{n+1}/P^n is currently of the order of 1/10 ($\forall \mu$ and ν), whereas the ratio K^{n+1}/K^n is not far from 1. In a practical sense, it is enough to calculate the first eight or ten functions for precisely evaluating P in the high-temperature domain $\tau^* < 10$ ($T > 2.7$ eV for two electrons).

The coefficients of the series

$$\tilde{A}_p^n(z) = \sum_{q \geqslant 0} \tilde{A}_{p,q}^n z^{q/2} \tag{31}$$

are then given by

$$\tilde{A}_{p,0}^n = \frac{1}{4p^3(p+1/2)} \tilde{A}_{p-1,0}^{n-2} + \frac{p+1/2-n/2}{p(p+1/2)} \tilde{A}_{p-1,0}^n$$

$$(p \geqslant 1, n \geqslant 0), \qquad \tilde{A}_{0,0}^n = \tilde{a}_0^n$$

$$\tilde{A}_{p,q}^n = -\frac{2}{q(q+2p+1)} \left[(q+2p+1-n)\, \tilde{A}_{p,q-2}^n + \tilde{A}_{p,q-1}^{n-1}\right] \tag{32}$$

$$(n \geqslant 0,\ p \geqslant 0,\ q \geqslant 1)$$

with the convention $\tilde{A}_{p,q}^n = 0$ for $n < 0$ or $q < 0$. It is possible to avoid multiplying by e^{μ^2}, (29), by drawing up the recurrences for the coefficients $A_{p,q}^n$

of the functions K^n. We shall give the formulas with extensive results. In the exchange case ($\mu = \nu$), we have

$$A^n(z) = e^z \tilde{A}^n(z) = \sum_{q \geqslant 0} a_q^n z^{q/2}, \qquad A^0(z) = 1$$

$$a_q^n = \frac{2}{q(q+1)} [(n+q-2)\, a_{q-2}^n - a_{q-1}^{n-1}] \qquad (n \geqslant 1, q \geqslant 1) \tag{33}$$

$$a_0^n = \tilde{a}_0^n, \qquad a_q^n = 0 \qquad (q < 0)$$

Finally, the self-function ($\mu = 0$) is given by

$$B^n(z) = \sum_{q \geqslant 0} b_q^n z^{q/2}, \qquad B^0(z) = 1$$

$$b_q^n = -\frac{2}{q^2(q+1)} [(q-2)(q+1-n)\, b_{q-2}^n + 2(q - \tfrac{1}{2})\, b_{q-1}^{n-1}] \qquad (n \geqslant 1, q \geqslant 1) \tag{34}$$

$$b_0^n = \tilde{a}_0^n, \qquad b_q^n = 0 \qquad (q < 0)$$

All these series converge for all z. The functions P^n are finite for all distances and tend to zero at large distances. The series in τ^*, truncated at a given order, give good results for any spatial configuration if the value at the origin is good. Of course, the number of terms which are needed increases with the value of τ^*.

7. GENERAL SOLUTION

The expansions of the first coefficients $\tilde{A}_{p,q}^n$ [from (32)] lead to the following expansion for the $\tilde{K}^n$:

$$\begin{aligned}
\tilde{K}^n(x, z) = {} & \tilde{a}_0^n - \tilde{a}_0^{n-1} \sqrt{z} + [\tfrac{1}{3}(n-3)\, \tilde{a}_0^n + \tfrac{1}{3} \tilde{a}_0^{n-2}]\, z \\
& - [\tfrac{2}{9}(n-4)\, \tilde{a}_0^{n-1} + \tfrac{1}{18} \tilde{a}_0^{n-3}]\, z^{3/2} + \cdots \\
& + x\{[-\tfrac{1}{3}(n-3)\, \tilde{a}_0^n + \tfrac{1}{6} \tilde{a}_0^{n-2}] \\
& + [\tfrac{1}{6}(n-4)\, \tilde{a}_0^{n-1} - \tfrac{1}{12} \tilde{a}_0^{n-3}] \sqrt{z} + \cdots\} \\
& + x^2\{[\tfrac{1}{30}(n-3)(n-5)\, \tilde{a}_0^n - \tfrac{1}{48} \tilde{a}_0^{n-2} + \tfrac{1}{480} \tilde{a}_0^{n-4}] + \cdots\} \\
& + \cdots
\end{aligned} \tag{35}$$

with $\tilde{a}_0^n = 0$ for $n < 0$; this suggests that $\tilde{K}_\tau(x, z)$ can be expressed as a function of $\tilde{K}_\tau(x = 0, z = 0) = \tilde{A}_\tau(z = 0)$ and of its derivatives with respect to τ^*.

Therefore, we come back to differential equations for $\tilde{K}_\tau$ in the variables (ξ, η) and introduce the expansion in powers of $\eta = 2\sqrt{\tau^*}\sqrt{x}$:

$$\tilde{K}_\tau(\xi, \eta) = \tau^{*3/2} \sum_{p \geq 0} \eta^{2p} \tilde{\mathscr{A}}_p(\tau^*, \xi), \qquad \tilde{A}_p = 2^{2p} \tau^{*p+3/2} \tilde{\mathscr{A}}_p \tag{36}$$

The differential equations (10) and (12) for $\tilde{K}_\tau$ lead to

$$\begin{gathered} \left(2\frac{p+1}{\xi}\frac{\partial}{\partial \xi} - \frac{\varepsilon}{\xi}\right) \tilde{\mathscr{A}}_p + 4(p+1)^2\, \tilde{\mathscr{A}}_{p+1} = 0 \\ \left(\frac{\partial}{\partial \tau^*} - \frac{\partial^2}{\partial \xi^2}\right) \tilde{\mathscr{A}}_p + 4(p+1)^2\, \tilde{\mathscr{A}}_{p+1} = 0 \end{gathered} \tag{37}$$

from which we deduce the function $\tilde{\mathscr{A}}_p(\tau^*, \xi)$,

$$\tilde{\mathscr{A}}_p(\tau^*, \xi) = \frac{1}{2^{2p}(p!)^2}\left(-\frac{\partial}{\partial \tau^*} + \frac{\partial^2}{\partial \xi^2}\right)^p \tilde{\mathscr{A}}(\tau^*, \xi) \tag{38}$$

in terms of the exchange function

$$\tilde{\mathscr{A}}(\tau^*, \xi) = \tilde{\mathscr{A}}_{p=0}(\tau^*, \xi) = \frac{\tilde{A}(\tau^*, z)}{\tau^{*3/2}}$$

The latter satisfies the differential equation

$$\left[\frac{\partial}{\partial \tau^*} - \left(\frac{\partial^2}{\partial \xi^2} + \frac{2}{\xi}\frac{\partial}{\partial \xi} - \frac{\varepsilon}{\xi}\right)\right] \tilde{\mathscr{A}}(\tau^*, \xi) = 0 \tag{39}$$

The series expansion

$$\tilde{\mathscr{A}}(\tau^*, \xi) = \sum_{q \geq 0} (\varepsilon \xi)^q\, \tilde{A}_q(\tau^*) \tag{40}$$

is then determined by

$$\begin{gathered} (q+2)(q+3)\, \tilde{A}_{q+2} = \tilde{A}_{q+1} + \frac{\partial}{\partial \tau^*} \tilde{A}_q \quad (q \geq -1), \qquad \tilde{A}_q = 0 \quad (q < 0) \\ \tilde{A}_0(\tau^*) = \frac{\tilde{A}(\tau^*, z=0)}{\tau^{*3/2}} = \frac{1}{\tau^{*3/2}} \sum_{n \geq 0} (-\varepsilon\sqrt{\tau^*})^n\, \tilde{a}_0^n = \frac{1}{\tau^{*3/2}} e^{-P_\tau(0,0)} \end{gathered} \tag{41}$$

Equations (38) and (41) give $\tilde{K}_\tau(\xi, \eta)$ as a series in ξ and η^2, with coefficients which are indeed functions only of $\tilde{A}_0(\tau^*)$ and its derivatives with respect to τ^*.

For the self-function, it is possible to avoid summing on p. In the same way as in Section 5, we deduce for the self-function

$$\mathscr{B} = \frac{B}{\tau^{*3/2}} = \sum_{q \geqslant 0} (\varepsilon\xi)^q M_q(\tau^*) \tag{42}$$

the third-order differential equation

$$\left[\frac{\partial^3}{\partial\xi^3} + \frac{4}{\xi}\frac{\partial^2}{\partial\xi^2} - \frac{\partial^2}{\partial\xi\,\partial\tau^*} + \left(\frac{2}{\xi^2} - 2\frac{\varepsilon}{\xi}\right)\frac{\partial}{\partial\xi} - \frac{\varepsilon}{\xi^2}\right]\mathscr{B}(\tau^*, \xi) = 0 \tag{43}$$

and the recurrence for the coefficients M_q

$$\begin{aligned}(q+3)^2(q+4)\,M_{q+3} &= (2q+5)\,M_{q+2} + (q+1)\frac{\partial}{\partial\tau^*}M_{q+1} \quad (q \geqslant -2)\\ M_q &= 0 \quad (q<0)\\ M_{q=0} &= \tilde{\Lambda}_0\end{aligned} \tag{44}$$

It must be noticed that the coefficients $\tilde{\Lambda}_q$ and M_q depend on ε as $\tilde{\Lambda}_0$.

8. VALUE AT THE ORIGIN

For low temperature, it is necessary to sum exactly the series (41) giving $\tilde{\Lambda}_0(\tau^*)$. This result is obtained by means of an integral. For that, we use Hankel's representation[11] for $\Gamma(n-1)/2$ which appears in the coefficient $\tilde{a}_0^n$ and the series expansion of $\psi(1+z)$ (psi function)[11] and we get

$$\begin{aligned}\tilde{\Lambda}_0(\tau^*) &= \frac{\tilde{\Lambda}(\tau^*, z=0)}{\tau^{*3/2}} = \int_C du\, F(u)\, e^{-\tau^* u}\\ F(u) &= \frac{i\varepsilon}{\sqrt{\pi}}\left[\psi\left(1 + \frac{i\varepsilon}{2\sqrt{u}}\right) - \psi(1) + i\varepsilon\sqrt{u} + \operatorname{Log} u\right]\end{aligned} \tag{45}$$

with the following branch definition of $\sqrt{u}$ and $\operatorname{Log} u$:

$$\sqrt{u} = \sqrt{\rho}\, e^{i\theta/2}, \qquad \operatorname{Log} u = \operatorname{Log}\rho + i\theta, \qquad u = \rho e^{i\theta} \qquad (0 < \theta < 2\pi) \tag{46}$$

The path C starts from $+\infty$ on the real axis, circles the point $u = -1/4$ in the counterclockwise direction, and returns to $+\infty$ by never crossing the real axis from $u = -1/4$ to $+\infty$. The ψ function in F exhibits for $\varepsilon = -1$, and only in that case, simple poles for $-i/2\sqrt{u} = -n$ $(n \geqslant 1)$. In the function $F(u)$, $i\varepsilon\sqrt{u}$ and $\operatorname{Log} u$ are the contributions of the terms $n = 0$ and

$n=1$ in the sum (41); the terms $n \geqslant 2$ precisely give the difference of the psi function. By isolating the contributions of the poles ($\varepsilon = -1$) and bringing together the contributions which result from the difference $F(u+i\alpha) - F(u-i\alpha)$ ($u>0$, $\alpha \to 0$), we obtain the integral

$$\int_C du\, f(u)\, F(u)\, e^{-\tau^* u} = \frac{1+\varepsilon}{2} \sqrt{\pi} \sum_{n \geqslant 1} \frac{1}{n^3} e^{\tau^*/4n^2} f\left(-\frac{1}{4n^2}\right) + 2\varepsilon \sqrt{\pi} \int_0^{+\infty} du \frac{e^{-\tau^* u}}{e^{\pi\varepsilon/\sqrt{u}} - 1} f(u) \tag{47}$$

of any function $f(u)$, which is assumed to be regular on and near the half real axis $u \geqslant -1/4$. We have used the formula giving $\operatorname{Im} \psi(1+iy)$ in terms of $\operatorname{th}(\pi y/2)$.[11] The first term ($\varepsilon = -1$) is the contribution of the bound states which exist in that case.

9. VALUE AT FINITE DISTANCE

It is easily seen that the functions which appear in the expansion of $\tilde{K}_\tau(\xi, \eta)$ can be written as integrals in the same form. From the recurrence $\tilde{A}_1 = \frac{1}{2}\tilde{A}_0$, $\tilde{A}_2 = \frac{1}{6}(\frac{1}{2}\tilde{A}_0 + \partial\tilde{A}_0/\partial\tau^*)$,..., we deduce

$$\tilde{A}_q = \int_C du\, F(u)\, e^{-\tau^* u} Q_q(u) \tag{48}$$

where the polynomials $Q_q(u)$ are defined by

$$(q+2)(q+3)\, Q_{q+2}(u) = Q_{q+1}(u) - u Q_q(u) \quad (q \geqslant 0), \qquad Q_0 = 1, \quad Q_1 = \tfrac{1}{2} \tag{49}$$

The function

$$Q(\varepsilon\xi, u) = \sum_{q \geqslant 0} Q_q(u) (\varepsilon\xi)^q, \qquad \tilde{\mathscr{A}} = \frac{\tilde{A}}{\tau^{*3/2}} = \int_C du\, F(u)\, e^{-\tau^* u} Q(\varepsilon\xi, u) \tag{50}$$

satisfies the differential equation

$$\left(\frac{\partial^2}{\partial\xi^2} + \frac{2}{\xi}\frac{\partial}{\partial\xi} - \frac{\varepsilon}{\xi} + u\right) Q(\varepsilon\xi, u) = 0 \tag{51}$$

In the same way, we get for the functions $\tilde{\mathscr{A}}_p$ and $\tilde{K}$

$$\tilde{\mathscr{A}}_p = \frac{\tilde{A}_p}{2^{2p}\tau^{*p+3/2}} = \int_C du\, F(u)\, e^{-\tau^* u} Q^p(\varepsilon\xi, u)$$

$$\frac{\tilde{K}_\tau}{\tau^{*3/2}} = \int_C du\, F(u)\, e^{-\tau^* u} R(\varepsilon\xi, \eta, u)$$

$$Q^p(\varepsilon\xi, u) = \sum_{q \geqslant 0} Q_q^p(u)(\varepsilon\xi)^q, \qquad R(\varepsilon\xi, \eta, u) = \sum_{p \geqslant 0} \eta^{2p} Q^p(\varepsilon\xi, u) \tag{52}$$

$$Q^p(\varepsilon\xi, u) = \frac{1}{2^{2p}(p!)^2}\left(\frac{\partial^2}{\partial\xi^2} + u\right)^p Q(\varepsilon\xi, u) \qquad (p \geqslant 0)$$

the recurrences

$$(q+2)(q+2p+3)\, Q_{q+2}^p(u) = Q_{q+1}^p(u) - uQ_q^p(u) \quad (p \geqslant 0, q > -2), \qquad Q_q^p = 0 \quad (q < 0) \tag{53}$$

$$Q_0^p(u) = \frac{Q_0^{p-1}(u)}{(2p)^3\,(2p+1)}(1 + 4p^2 u) \quad (p \geqslant 1), \qquad Q_0^0 = 1$$

and the differential equations

$$\left(\frac{\partial^2}{\partial\xi^2} + 2\frac{p+1}{\xi}\frac{\partial}{\partial\xi} - \frac{\varepsilon}{\xi} + u\right) Q^p(\varepsilon\xi, u) = 0$$

$$-uR = \left[\frac{\partial^2}{\partial\xi^2} - \left(\frac{\partial^2}{\partial\eta^2} + \frac{1}{\eta}\frac{\partial}{\partial\eta}\right)\right] R = \left(\frac{\partial^2}{\partial\xi^2} + \frac{2}{\xi}\frac{\partial}{\partial\xi} - \frac{\varepsilon}{\xi} + \frac{\eta}{\xi}\frac{\partial^2}{\partial\xi\,\partial\eta}\right) R \tag{54}$$

It is easily seen that $Q_{2q}^p(u)$ and $Q_{2q+1}^p(u)$ are polynomials of degree $p+q$ in u.

Finally, in the self case these formulas are

$$M_q = \int_C du\, F(u)\, e^{-\tau^* u} S_q(u) \tag{55}$$

$$(q+3)^2\,(q+4)\, S_{q+3}(u) = (2q+5)\, S_{q+2}(u) - (q+1)\, uS_{q+1}(u)$$

$$S_0 = 1, \qquad S_q = 0 \qquad (q < 0) \tag{56}$$

$$\frac{B}{\tau^{*3/2}} = \int_C du\, F(u)\, e^{-\tau^* u} S(\varepsilon\xi, u), \qquad S(\varepsilon\xi, u) = \sum_{q \geqslant 0} S_q(u)(\varepsilon\xi)^q \tag{57}$$

$$\left[\frac{\partial^3}{\partial\xi^3} + \frac{4}{\xi}\frac{\partial^2}{\partial\xi^2} + u\frac{\partial}{\partial\xi} + \left(\frac{2}{\xi^2} - \frac{2\varepsilon}{\xi}\right)\frac{\partial}{\partial\xi} - \frac{\varepsilon}{\xi^2}\right] S(\varepsilon\xi, u) = 0 \tag{58}$$

$S_{2q+2}(u)$ and $S_{2q+1}(u)$ are polynomials of degree q in u.

10. INTEGRAL REPRESENTATION

By using Laplace transformation for the differential equation (51), we deduce the following integral representation of the function $Q(\varepsilon\xi, u)$:

$$Q(\varepsilon\xi, u) = \frac{\sqrt{u}}{2\pi i} \oint dt \exp\left(-\frac{i}{2\sqrt{u}} \operatorname{Log} \frac{t+i}{t-i} + \varepsilon\xi\sqrt{u}\, t\right) \tag{59}$$

Integration is made on a closed contour encircling, and not crossing, the branch line $t = it_2$ $(-1 \leqslant t_2 \leqslant 1)$ of the logarithm. The branch definition for that function is

$$\operatorname{Log} \frac{t+i}{t-i} = \operatorname{Log} \frac{r_1}{r_2} + i(\varphi_1 - \varphi_2), \qquad t + i = r_1 e^{i\varphi_1}, \qquad t - i = r_2 e^{i\varphi_2} \tag{60}$$

and $\sqrt{u}$ is defined in (46) for complex u.

The function $Q^p(\varepsilon\xi, u)$ of (52) follows by derivating (59), and summing the series in η^{2p}, we get for $R(\varepsilon\xi, \eta, u)$

$$\begin{aligned} R(\varepsilon\xi, \eta, u) = \frac{\sqrt{u}}{2\pi i} \oint dt &\left[\exp\left(-\frac{i}{2\sqrt{u}} \operatorname{Log} \frac{t+i}{t-i} + \varepsilon\xi\sqrt{u}\, t\right)\right] \\ &\times I_0(\eta\sqrt{u}\,(1+t^2)^{1/2}) \end{aligned} \tag{61}$$

with the same contour, and the same branch definition of $\operatorname{Log}[(t+i)/(t-i)]$ and $\sqrt{u}$ as in (59); I_0 is the Bessel function,[11] which is an entire function of $\eta^2 u(1+t^2)$, so that the branch definition of $(1+t^2)^{1/2}$ is not relevant. This formula gives, with (52), the density matrix as a double integral, which is valid for all values of ε, τ^*, ξ, and η. This result has been obtained by successively summing the three series in τ^*, ξ, and η. For integrating on u, see (47).

11. SOME APPLICATIONS

All these results allow us to get numerical values of P and small- and large-distance expansions. Here we give some examples. From (52), the expansion of $P_\tau(\xi, \eta)$ is written in the form

$$\begin{aligned} &\exp\left\{-\left[P_\tau(\xi, \eta) - P_\tau(0, 0) + \frac{\xi^2 - \eta^2}{4\tau^*}\right]\right\} \\ &\quad = 1 + \sum_{\substack{p, q \geqslant 0 \\ 2p + q \neq 0}} \eta^{2p} (\varepsilon\xi)^q \, \overline{Q_q^p(u)} \end{aligned} \tag{62}$$

where $\overline{f(u)}$ stands for the mean value of $f(u)$ on C,

$$\overline{f(u)} = \int_C du\, f(u)\, F(u)\, e^{-\tau^* u} \Big/ \int_C du\, F(u)\, e^{-\tau^* u} \tag{63}$$

As the polynomials $Q_q^p(u)$ are quite simple, the first coefficients depend on τ^* through the mean value $\bar{u}(\tau^*, \varepsilon)$ and the variance $\overline{\Delta u^2}(\tau^*, \varepsilon)$. In this way, we get the expansion of $P_\tau(\xi, \eta)$ to the fourth order in $\varepsilon\xi$ and η, valid for all temperatures:

$$\begin{aligned}
&P_\tau(\xi, \eta) - P_\tau(0, 0)\\
&\quad = -\frac{1}{2}(\varepsilon\xi) + \frac{1}{24}\left(1 + 4\bar{u} - \frac{6}{\tau^*}\right)(\xi^2 - \eta^2) + \frac{1}{48}(1 + 4\bar{u})\,\varepsilon\xi\left(\frac{1}{2}\eta^2 - \frac{1}{3}\xi^2\right)\\
&\qquad + \frac{1}{3!\,5!}\left[(1 + 4\bar{u})(1 + \bar{u}) - 6\,\overline{\Delta u^2}\right]\xi^2(\xi^2 - 2\eta^2)\\
&\qquad + \frac{1}{4^2(2!)^2\,5!\,3}\left[(1 + 4\bar{u})(17 + 32\bar{u}) - 192\,\overline{\Delta u^2}\right]\eta^4
\end{aligned} \tag{64}$$

The functions $P_\tau(0, 0), \bar{u}, \ldots$ are related to $\tilde{\Lambda}_0(\tau^*)$ by

$$\begin{aligned}
P_\tau(0, 0) &= -\text{Log}\,\tilde{\Lambda}_0 - \frac{3}{2}\,\text{Log}\,\tau^*, \qquad \bar{u} = -\frac{\partial}{\partial\tau^*}\,\text{Log}\,\tilde{\Lambda}_0\\
\overline{\Delta u^2} &= \frac{\partial^2}{\partial\tau^{*2}}\,\text{Log}\,\tilde{\Lambda}_0
\end{aligned} \tag{65}$$

The high-temperature ($\tau^* < 1$) expansions of these functions are easily obtained from (41). In the low-temperature limit ($\tau^* \gg 1$), we get from (45) with (47) the expansions

$$\begin{aligned}
-\text{Log}\,\tilde{\Lambda}_0 &\sim 3\left(\frac{\pi}{2}\right)^{2/3}\tau^{*1/3} - \text{Log}\left[\frac{8}{\sqrt{3}}\left(\frac{\pi}{2}\right)^{4/3}\right] + \frac{5}{6}\,\text{Log}\,\tau^* \qquad (\varepsilon = +1)\\
-\text{Log}\,\tilde{\Lambda}_0 &\sim -\frac{1}{4}\tau^* - \text{Log}\sqrt{\pi} \qquad (\varepsilon = -1)
\end{aligned} \tag{66}$$

Therefore, in this limit, $\bar{u}$ tends to 0 for $\varepsilon = +1$, and to $-1/4$ for $\varepsilon = -1$; the moments $\overline{\Delta u^2}, \ldots$ tend to 0 in both cases. Thus, it appears that the difference $P_\tau(\xi, \eta) - P_\tau(0, 0)$ tends to a finite limit as the temperature decreases. In the attractive case, the corresponding contributions come from the ground state ($n = 1$); $\tilde{K}$ is then proportional to $R(-\xi, \eta, u = -1/4)$. In the repulsive case, $\tilde{K}$ becomes proportional to $R(\xi, \eta, u = 0)$.

At large distances, the behavior of P, of course, depends again on the temperature.

The large-distance expansion of $P_\tau(\xi, \xi)$ (self case) is easily obtained from the differential equation (43). The solution $\mathscr{B} = \tau^{*3/2} e^{-P}$, such that P tends to zero as ξ tends to infinity, is

$$P_\tau(\xi, \xi) \simeq \tau^* X - \frac{1}{12}\tau^{*3} X^4 - \frac{1}{15} X^6 \tau^{*4} + \left(-\frac{3}{28} X^8 + \frac{1}{30} X^7\right)\tau^{*5} + \left(-\frac{4}{15} X^{10} + \frac{88}{945} X^9\right)\tau^{*6} \quad (67)$$

$$X \equiv \frac{2\varepsilon}{\xi}$$

valid for $\xi/2 \gtrsim \tau^{*2/3}$ when $\tau^* > 1$, and $\xi/2 \gtrsim \sqrt{\tau^*}$ when $\tau^* < 1$. The first term of this asymptotic series is the Coulomb potential, and the following terms are Wigner–Kirkwood corrections, which appreciably improve the precision.

In the exchange case, the large-distance expansion of P is obtained from (21) and (22) in the form

$$P_\tau(\xi, \eta = 0) \simeq \sum_{p \geqslant 1} \tau^{*p} \left\{ \sum_{m=0}^{p-1} (1)^{p-1-m} P_m^{p-m}(Y)\, X^{p+m} \right\}$$
$$X \equiv \frac{2\varepsilon}{\xi}, \qquad Y = \operatorname{Log}\frac{\xi^2}{\tau^*} + \gamma \quad (68)$$

where γ is Euler's constant and the coefficients P_m^p are polynomials in Y. The first polynomials are given by

$$P_0^1 = \tfrac{1}{2} Y, \qquad P_1^1 = \tfrac{1}{4}, \qquad P_0^2 = \tfrac{1}{8}\varsigma(2)$$
$$P_2^1 = -\tfrac{3}{16}, \qquad P_1^2 = -\tfrac{1}{16}[Y^2 - 2Y + 2 + \varsigma(2)], \qquad P_0^3 = \tfrac{1}{24}\varsigma(3) \quad (69)$$
$$P_3^1 = \tfrac{5}{16}, \qquad P_2^2 = \tfrac{1}{32}[3Y^2 - 13Y + \tfrac{29}{2} + 3\varsigma(2)]$$
$$P_1^3 = \tfrac{1}{16}[-\varsigma(2)\, Y + \varsigma(2) - \varsigma(3)], \qquad P_0^4 = \tfrac{1}{64}\varsigma(4)$$

This expansion is valid for $\xi/2 \gtrsim \tau^*$ when $\tau^* > 1$, and $\xi/2 \gtrsim \sqrt{\tau^*}$ when $\tau^* < 1$.

In Table I, we compare results for $P_\tau(\xi, \xi)$ (self case) for $\tau^* = 10$ and $\varepsilon = +1$, calculated by the series expansion (34) with $n = 8$, by the integral (57) [the function $S(\xi, u)$ being obtained by summing the series], by the

Table I. Calculations of $P_\tau(\xi, \xi)$ (Self-Case) for $\tau^* = 10$, $\epsilon = +1$[a]

$\xi/2$	Series	Integral	Small-ξ expansion	Large-ξ expansion
0	5.0138	5.013861	5.013861	
0.2	4.8144	4.814377	4.814377	
0.4	4.6177	4.617686	4.617686	
0.6	4.4258	4.425809	4.425809	
0.8	4.2401	4.240091	4.240090	
1	4.0613	4.061362	4.061372	
1.5	3.6474	3.647531	3.648627	
2	3.2811	3.281137	3.301162	
2.5	2.9596	2.959366		
3	2.6785	2.677934		
4	2.2182	2.218010		2.156637
5	1.8677	1.867807		1.860152
6	1.5995	1.599628		1.598541
7	1.3919	1.391910		1.391776
8	1.2285	1.228525		1.228516
9	1.0978	1.097767		1.097770
10	0.9913	0.991292		0.991294

[a] Series expansion [Eq. (34)] with $n = 8$; integral [Eq. (57)]; small-distance expansion performed to the order 8 in ξ [as in Eq. (64)]; and large-distance expansion [Eq. (67)]. The accuracy is lower in the calculation by series than by integral because the number (eight) of functions P^n that we have kept is barely enough for that value of τ^*.

small-distance expansion of P_τ in (64), which we performed up to the order 8 in ξ, and finally by the large-distance expansion (67).

In Table II, some values of $P_\tau(\xi, \eta)$ are given for $\tau^* = 1$ and $\varepsilon = -1$ by using the series expansion (32) with $n = 8$. The limits $\mu/\nu = (1 - \eta^2/\xi^2)^{1/2} = 0$ and 1, respectively, correspond to the self and exchange cases. The variations of P_τ increase when μ/ν tends to one.

Table II. Values of $P_\tau(\xi, \eta)$ for $\tau^* = 1$, $\epsilon = -1$ Calculated by Series Expansion [Eq. (32)] with $n = 8$

$\xi/2$	$(1-\eta^2/\xi^2)^{1/2} = 0$	$= 0.2$	$= 0.4$	$= 0.6$	$= 0.8$	$= 1$
0	−1.85282	−1.85282	−1.85282	−1.85282	−1.85282	−1.85282
0.1	−1.75291	−1.75309	−1.75363	−1.75454	−1.75581	−1.75744
0.5	−1.36532	−1.36869	−1.37889	−1.39613	−1.42079	−1.45341
1	−0.95639	−0.96418	−0.98833	−1.03134	−1.09774	−1.19482
1.5	−0.67583	−0.68434	−0.71174	−0.76447	−0.85675	−1.01758
2	−0.50602	−0.51309	−0.53646	−0.58448	−0.68017	−0.88944
2.5	−0.40256	−0.40819	−0.42695	−0.46663	−0.55301	−0.79259
3	−0.33450	−0.33913	−0.35458	−0.38740	−0.46164	−0.71675

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