

## **Pair Correlation Function in a Dense Plasma and Pycnonuclear Reactions in Stars**

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*Received May 31, 1977*

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The short-range behavior of the pair correlation function in a dense one-component plasma (jellium) is investigated. As an intermediate step, the short-range behavior of the classical pair correlation function is obtained. Actually, although the temperature and the density are assumed to be such that the thermodynamic properties are almost classical, quantum mechanics (tunnel effect) always dominates the pair correlation function at short distances. The quantum pair correlation function is calculated by treating the many-body quantum effects by a perturbation theory, and by using a semiclassical approximation based on path integrals. The results are applied to the computation of the nuclear reaction rate in dense stellar matter (pycnonuclear reactions).

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**KEY WORDS:** One-component plasma ; pair correlation function (radial distribution function) ; quantum effects ; pycnonuclear reactions.

### **1. INTRODUCTION**

In this paper, we investigate the short-range behavior of the pair correlation function for the fluid phase of the one-component plasma. This model, also referred to as "jellium," a system of identical particles of charge  $Ze$  and mass  $M$  embedded in a uniform neutralizing background of opposite charge, has been shown to have well-behaved thermodynamic properties.<sup>(1)</sup> Jellium is believed to provide a good description of certain stellar interiors, where the nuclei are the particles and the degenerate electrons form the background. The knowledge of the pair correlation function at short distances is of importance, because it governs the rate of nuclear reactions, which is proportional to the probability that two nuclei approach one another at a distance of the order of the nuclear radius. In a dense plasma, strong screening effects increase the pair correlation function, and the rate of nuclear reactions is

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enhanced; the calculation of the enhancement factor has been of concern to several authors.<sup>(2-5)</sup>

The state of the plasma is defined by the number density  $\rho$  and the temperature  $T$ , or equivalently the ion-sphere radius  $a = (3/4\pi\rho)^{1/3}$  and the two-body average classical distance of closest approach  $\beta(Ze)^2$  ( $\beta = 1/kT$ , where  $k$  is Boltzmann's constant). The classical properties depend on the dimensionless parameter  $\Gamma = \beta(Ze)^2/a$ . We shall be primarily interested in the high-density regime  $1 \lesssim \Gamma \lesssim 155$  (for  $\Gamma \gtrsim 155$  the system becomes solid<sup>(6)</sup>). Throughout this paper, we shall assume the thermal de Broglie wavelength  $\lambda = (2\pi\hbar^2/MkT)^{1/2}$  to be small compared to the ion-sphere radius  $a$ . Note that the simultaneous requirements  $\lambda/a < 1$  and  $\Gamma > 1$  imply that the temperature must be neither too low nor too high. The assumption that  $\lambda$  is small ensures that the thermodynamic properties of the plasma can be essentially computed by classical statistical mechanics; small quantum corrections to the thermodynamic properties<sup>(7)</sup> can thereafter be obtained by a Wigner-Kirkwood expansion<sup>(8)</sup> in powers of  $\hbar^2$ . The Wigner-Kirkwood expansion can also be used for computing quantum corrections to the pair correlation function<sup>(9)</sup>  $g(r)$ , if the distance  $r$  is large enough. However, for the small values of  $r$  in which we are interested here, the pair correlation function is governed by quantum effects, which are no longer corrections and *cannot* be obtained by a Wigner-Kirkwood expansion. This is particularly evident in the extreme case of zero distance, where the classical Boltzmann factor  $\exp(-\beta Z^2 e^2/r)$  gives a vanishing classical pair correlation function, although quantum tunneling makes the true pair correlation function finite.

When two particles 1 and 2 are at short distance  $r$  from one another, the Wigner-Kirkwood expansion for  $g(r)$  fails because its coefficients involve derivatives of the potential, the direct interaction part  $(Ze)^2/r$  of which becomes singular. The other terms in the potential (interactions of 1 and 2 with other particles, and interactions of other particles with one another), however, remain regular, of order  $(Ze)^2/a$ , for all the configurations that have a nonnegligible statistical weight. Therefore, one is led to devise a method of approximation that may be considered as a modified Wigner-Kirkwood expansion adapted to the present case. In zeroth order, particles 1 and 2 are treated by quantum statistical mechanics, whereas all other particles are treated by classical statistical mechanics. Corrections to this zeroth-order approximation are thereafter expanded in a systematic way in powers of  $\hbar$ . This approximation scheme allows the quantum pair correlation function to be expressed in terms of classical quantities. It is therefore possible to use the known results about the classical system, obtained by computer simulation<sup>(10-12)</sup> or through the hypernetted chain approximation.<sup>(12-15)</sup>

The classical pair correlation function will be studied in Section 2. In Section 3, the calculation of the quantum pair correlation function will be

approximately reduced to a two-body problem. In Section 4, this two-body problem will be solved, through the use of the semiclassical approximation derived from the path integral formalism. Exchange terms will be neglected; a partial justification for this neglect will be given in Section 5. Finally, the results and their application to the problem of the nuclear reaction rate enhancement will be discussed in Section 6.

## 2. CLASSICAL PAIR CORRELATION FUNCTION

In this section, as an introductory step, we study the short-range behavior of the *classical* pair correlation function.

The potential energy for  $N$  particles of charge  $Ze$ , plus the background, in a volume  $\Omega$ , is

$$\begin{aligned}
 V(\mathbf{r}_1, \dots, \mathbf{r}_N) &= \sum_{1 \leq i < j \leq N} \frac{(Ze)^2}{r_{ij}} - (Ze)^2 \rho \sum_{1 \leq i \leq N} \int \frac{d\mathbf{r}}{|\mathbf{r}_i - \mathbf{r}|} + \frac{(Ze)^2}{2} \rho^2 \int \frac{d\mathbf{r} d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \\
 &= \frac{(Ze)^2}{r_{12}} + W(\mathbf{r}_1, \dots, \mathbf{r}_N)
 \end{aligned}
 \tag{1}$$

$W$  is the sum of all interactions except the one between particles 1 and 2. For the evaluation of the classical pair correlation function  $g_c(r_{12})$  at small separations  $r_{12}$ , we can choose both  $r_1$  and  $r_2$  to be small, and the contribution of  $W$  to the Boltzmann factor can be replaced by its Taylor expansion with respect to  $\mathbf{r}_1$  and  $\mathbf{r}_2$ ; grouping equivalent terms gives, to second order in  $\mathbf{r}_1$  and  $\mathbf{r}_2$ ,

$$\begin{aligned}
 \exp(-\beta V) &= \exp\left[\frac{-\beta(Ze)^2}{r_{12}}\right] \exp[-\beta W(0, 0, \mathbf{r}_3, \dots, \mathbf{r}_N)] \\
 &\times \left\{ 1 - \beta \frac{\partial W}{\partial \mathbf{r}_1} \cdot (\mathbf{r}_1 + \mathbf{r}_2) - \frac{\beta}{2} \frac{\partial^2 W}{\partial \mathbf{r}_1 \partial \mathbf{r}_1} : (\mathbf{r}_1 \mathbf{r}_1 + \mathbf{r}_2 \mathbf{r}_2) \right. \\
 &\left. + \frac{\beta^2}{2} \left[ \frac{\partial W}{\partial \mathbf{r}_1} \cdot (\mathbf{r}_1 + \mathbf{r}_2) \right]^2 + \dots \right\}
 \end{aligned}
 \tag{2}$$

where the derivatives of  $W$  are taken at the configuration-space point  $(0, 0, \mathbf{r}_3, \dots, \mathbf{r}_N)$ . Taking into account the invariance of  $W(0, 0, \mathbf{r}_3, \dots, \mathbf{r}_N)$  under rotations around the origin, we find for the pair correlation function

$$\begin{aligned}
 g_c(r_{12}) &= \frac{N(N-1)}{\rho^2 Q} \int \exp(-\beta V) d\mathbf{r}_3 \dots d\mathbf{r}_N \\
 &= \exp\left[\frac{-\beta(Ze)^2}{r_{12}}\right] \frac{N(N-1)}{\rho^2 Q} \int \exp[-\beta W(0, 0, \mathbf{r}_3, \dots, \mathbf{r}_N)] \\
 &\times \left[ 1 - \frac{\beta}{6} (\Delta_1 W)(r_1^2 + r_2^2) + \frac{\beta^2}{6} \left( \frac{\partial W}{\partial \mathbf{r}_1} \right)^2 (\mathbf{r}_1 + \mathbf{r}_2)^2 + \dots \right] d\mathbf{r}_3 \dots d\mathbf{r}_N
 \end{aligned}
 \tag{3}$$

where  $Q$  is the configuration integral

$$Q = \int \exp(-\beta V) d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N \quad (4)$$

Several useful remarks can be made about the quantities appearing in (3):

(a) Let us put

$$U(\mathbf{r}_1, \mathbf{r}_3, \dots, \mathbf{r}_N) = W(\mathbf{r}_1, \mathbf{r}_1, \mathbf{r}_3, \dots, \mathbf{r}_N) \quad (5)$$

$U$  is the potential energy of a system  $S'$  made up of one charge  $2Ze$  at  $\mathbf{r}_1$ ,  $N - 2$  charges  $Ze$  at  $\mathbf{r}_3, \dots, \mathbf{r}_N$ , and a neutralizing background, in a volume  $\Omega$ ; the configuration integral of this system is

$$\begin{aligned} Q' &= \int \exp[-\beta U(\mathbf{r}_1, \mathbf{r}_3, \dots, \mathbf{r}_N)] d\mathbf{r}_1 d\mathbf{r}_3 \cdots d\mathbf{r}_N \\ &= \Omega \int \exp[-\beta W(0, 0, \mathbf{r}_3, \dots, \mathbf{r}_N)] d\mathbf{r}_3 \cdots d\mathbf{r}_N \end{aligned} \quad (6)$$

and

$$Q'/Q = \Omega^{-1} \exp[\beta F(0, N) - \beta F(1, N - 2)] \quad (7)$$

where  $F(M, N)$  is the excess free energy of a mixture of  $M$  charges  $2Ze$  and  $N$  charges  $Ze$ .

(b) The Laplacian

$$\Delta_1 W(0, 0, \mathbf{r}_3, \dots, \mathbf{r}_N) = -4\pi(Ze)^2 \sum_{j=3}^N \delta(\mathbf{r}_j) + 4\pi(Ze)^2 \rho \quad (8)$$

is multiplied in (3) by  $\exp(-\beta W)$ , which vanishes at  $r_j = 0$ . Therefore, only the background term  $4\pi(Ze)^2 \rho$  of (8) contributes to (3).

(c) The term involving the gradient  $\partial W/\partial \mathbf{r}_1$  in (3) can be evaluated as follows. The mean square force acting on the particle 1 of the system  $S'$  is obtained by integration by parts:

$$\begin{aligned} &\frac{1}{Q'} \int \exp[-\beta U(\mathbf{r}_1, \mathbf{r}_3, \dots, \mathbf{r}_N)] \left( \frac{\partial U}{\partial \mathbf{r}_1} \right)^2 d\mathbf{r}_1 d\mathbf{r}_3 \cdots d\mathbf{r}_N \\ &= \frac{1}{\beta Q'} \int \exp(-\beta U) \Delta_1 U d\mathbf{r}_1 d\mathbf{r}_3 \cdots d\mathbf{r}_N = 8\pi(Ze)^2 \rho kT \end{aligned} \quad (9)$$

since only the background term  $8\pi(Ze)^2 \rho$  of  $\Delta_1 U$  contributes to  $\exp(-\beta U) \Delta_1 U$ . Using (5) in (9), we find

$$\begin{aligned} \left\langle \left( \frac{\partial W}{\partial \mathbf{r}_1} \right)^2 \right\rangle &= \frac{\Omega}{Q'} \int \exp[-\beta W(0, 0, \mathbf{r}_3, \dots, \mathbf{r}_N)] \left( \frac{\partial W}{\partial \mathbf{r}_1} \right)^2 d\mathbf{r}_3 \cdots d\mathbf{r}_N \\ &= 2\pi(Ze)^2 \rho kT \end{aligned} \quad (10)$$

Using the above remarks, we obtain from (3)

$$g_c(r_{12}) = \exp\left[-\frac{\beta(Ze)^2}{r_{12}} + C\right] \left[1 - \beta \frac{\pi(Ze)^2 \rho}{3} r_{12}^2 + \dots\right] \tag{11}$$

or equivalently, to order  $r^2$ ,

$$g_c(r) = \exp\left[-\frac{\beta(Ze)^2}{r} + C - \beta \frac{\pi(Ze)^2 \rho}{3} r^2 + \dots\right] \tag{12}$$

where

$$C = \beta[F(0, N) - F(1, N - 2)] \tag{13}$$

Since (12) results from the expansion (11), Eq. (12) will be valid if

$$\beta(Ze)^2 \rho r^2 \ll 1 \quad \text{or equivalently} \quad \Gamma(r/a)^2 \ll 1 \tag{14}$$

The  $r^2$  contribution to the potential of mean force in (12) can be given a simple interpretation if we assume the background to be a large sphere centered at the origin and the particles 1 and 2 to be located at the symmetric points  $r/2$  and  $-r/2$ ; then the sum of the interaction energies between each of these particles and the background<sup>2</sup> depends on  $r$  as  $\pi(Ze)^2 \rho r^2/3$ .

An evaluation of the constant  $C$  has been made by DeWitt *et al.*,<sup>(4)</sup> using computer simulation results<sup>(10)</sup> for the one-component plasma pair correlation function  $g_c(r)$ . Computer results unfortunately are not available for those small values of  $r$  that make (12) valid [because the computed  $g_c(r)$ <sup>(10,11)</sup> is indistinguishable from zero in that region], and an extrapolation method had to be used. However,  $C$  can now be computed from (13), since recent numerical results on mixtures have been obtained by Hansen *et al.*<sup>(12,15)</sup> They have given a good approximation for the excess free energy  $F(M, N)$ , which is, in our notation,

$$\beta F(M, N) = N f_0 \left[ \Gamma \left( \frac{N + 2M}{N} \right)^{1/3} \right] + M f_0 \left[ \Gamma \left( \frac{N + 2M}{N} \right)^{1/3} 2^{5/3} \right] \tag{15}$$

where  $kTf_0(\Gamma)$  is the excess free energy per particle of a one-component plasma of charges  $Ze$ ; the computer results<sup>(11)</sup> for  $f_0$  are well fitted in the range  $1 \lesssim \Gamma \lesssim 155$  by<sup>(16,12)</sup>

$$f_0(\Gamma) = -0.896434\Gamma + 3.44740\Gamma^{1/4} - 0.5551 \ln \Gamma - 2.996 \tag{16}$$

<sup>2</sup> DeWitt *et al.*<sup>(4)</sup> have derived an expression similar to (12), with, however, a coefficient of  $r^2$  that is twice ours. We believe they have violated the symmetry of the problem by assuming the background to be a sphere centered at one of the two particles rather than at their center of mass.

Using (15) and (16) in (13), we obtain

$$\begin{aligned} C &= 2f_0(\Gamma) - f_0(2^{5/3}\Gamma) \\ &= 1.0531\Gamma + 2.2931\Gamma^{1/4} - 0.5551 \ln \Gamma - 2.35 \end{aligned} \quad (17)$$

in reasonable agreement with the more uncertain values obtained by an extrapolation of the computer results for  $g_c(r)$ .

### 3. QUANTUM PAIR CORRELATION FUNCTION

In quantum statistical mechanics, the formal expression for the pair correlation function is

$$g(r_{12}^0) = \frac{N(N-1)}{\rho^2} \frac{\int \langle \mathbf{r}_1^0 \dots \mathbf{r}_N^0 | \exp(-\beta H) | \mathbf{r}_1^0 \dots \mathbf{r}_N^0 \rangle d\mathbf{r}_3^0 \dots d\mathbf{r}_N^0}{\int \langle \mathbf{r}_1^0 \dots \mathbf{r}_N^0 | \exp(-\beta H) | \mathbf{r}_1^0 \dots \mathbf{r}_N^0 \rangle d\mathbf{r}_1^0 d\mathbf{r}_2^0 d\mathbf{r}_3^0 \dots d\mathbf{r}_N^0} \quad (18)$$

In (18), the exchange effects are not taken into account; a partial justification for this neglect will be given in Section 5. It is convenient to split the total Hamiltonian  $H$  into

$$H = H_0 + W \quad (19)$$

$W$  is defined by (1) and  $H_0$  by

$$H_0 = -\frac{\hbar^2}{2M} \sum_{i=1}^N \Delta_i + \frac{(Ze)^2}{r_{12}} \quad (20)$$

In all regions of configuration space that significantly contribute to the denominator of (18), the potentials are regular, and therefore this denominator can be related to the Wigner-Kirkwood expansion of the free energy<sup>(11,7)</sup>; to order  $\hbar^2$ ,

$$\begin{aligned} &\int \langle \mathbf{r}_1^0 \dots \mathbf{r}_N^0 | \exp(-\beta H) | \mathbf{r}_1^0 \dots \mathbf{r}_N^0 \rangle d\mathbf{r}_1^0 \dots d\mathbf{r}_N^0 \\ &= \lambda^{-3N} Q \left[ 1 - N \frac{\hbar^2 \beta^2 \pi (Ze)^2 \rho}{6M} \right] \end{aligned} \quad (21)$$

where  $Q$  is the classical configuration integral (4).

For the numerator of (18), as explained in the introduction, we must use a modified expansion, which allows for the singularity of  $(Ze)^2/r_{12}$  in (20), since we are precisely interested in small  $r_{12}$  values. However,  $W$  is regular in all regions of configuration space that significantly contribute to the numerator of (18), and we can replace  $W$  by its Taylor expansion to second order around the configuration-space point  $(0, 0, \mathbf{r}_3^0, \dots, \mathbf{r}_N^0)$ ; since  $H$  is not diagonal in configuration space, we must now expand  $W$  with respect to *all*

coordinates. To second order in the coordinates, we obtain

$$\begin{aligned} \exp(-\beta H) = & \exp[-\beta W(0, 0, \mathbf{r}_3^0, \dots, \mathbf{r}_N^0)] \left\{ \exp(-\beta H_0) \right. \\ & - \int_0^\beta d\tau \exp[-(\beta - \tau)H_0] \left[ \sum_{i=1}^N \frac{\partial W}{\partial \mathbf{r}_i} \cdot (\mathbf{r}_i - \mathbf{R}_i) \right. \\ & + \left. \frac{1}{2} \sum_{i,j=1}^N \frac{\partial^2 W}{\partial \mathbf{r}_i \partial \mathbf{r}_j} : (\mathbf{r}_i - \mathbf{R}_i)(\mathbf{r}_j - \mathbf{R}_j) \right] \exp(-\tau H_0) \\ & + \int_0^\beta d\tau \int_0^\tau d\sigma \exp[-(\beta - \tau)H_0] \left[ \sum_{i=1}^N \frac{\partial W}{\partial \mathbf{r}_i} \cdot (\mathbf{r}_i - \mathbf{R}_i) \right] \\ & \times \exp[-(\tau - \sigma)H_0] \left[ \sum_{j=1}^N \frac{\partial W}{\partial \mathbf{r}_j} \cdot (\mathbf{r}_j - \mathbf{R}_j) \right] \exp(-\sigma H_0) \left. \right\} \quad (22) \end{aligned}$$

where  $\mathbf{R}_1 = \mathbf{R}_2 = 0$  and  $\mathbf{R}_i = \mathbf{r}_i^0$  ( $i = 3, \dots, N$ ). In (22), since

$$W(0, 0, \mathbf{r}_3^0, \dots, \mathbf{r}_N^0)$$

is a  $c$ -number,  $\exp(-\beta W)$  could be factorized out; the derivatives of  $W$  have to be taken at the point  $(0, 0, \mathbf{r}_3^0, \dots, \mathbf{r}_N^0)$  and are also  $c$ -numbers. In the numerator of (18), some terms from (22) vanish because of the rotational invariance of  $W(0, 0, \mathbf{r}_3^0, \dots, \mathbf{r}_N^0)$  and of  $H_0$ . In the remaining matrix elements, the contributions of the center of mass of particles 1 and 2 and the contributions of particles 3 to  $N$  can be factorized out and explicitly computed (the expansion with respect to these coordinates will generate an expansion in powers of the thermal wavelength  $\lambda$ ). Furthermore, for the derivatives of  $W$  appearing in (22), we can again use (8), (10), and similar expressions for the derivatives with respect to the other coordinates. Finally, the numerator of (18) becomes (for brevity, we sometimes drop the subscripts 1, 2, and call  $r$  the relative coordinate  $r_{12}$  and  $\Delta$  the corresponding Laplacian)

$$\begin{aligned} & \int \langle \mathbf{r}_1^0 \dots \mathbf{r}_N^0 | \exp(-\beta H) | \mathbf{r}_1^0 \dots \mathbf{r}_N^0 \rangle d\mathbf{r}_3^0 \dots d\mathbf{r}_N^0 \\ & = \left\{ \int \exp[-\beta W(0, 0, \mathbf{r}_3^0, \dots, \mathbf{r}_N^0)] d\mathbf{r}_3^0 \dots d\mathbf{r}_N^0 \right\} \\ & \times \frac{2^{3/2}}{\lambda^{3(N-1)}} \left\{ \left\langle \mathbf{r}_{12}^0 \left| \exp \left[ -\beta \left( -\frac{\hbar^2}{M} \Delta + \frac{Z^2 e^2}{r} \right) \right] \right| \mathbf{r}_{12}^0 \right\rangle \right. \\ & \times \left[ 1 - (N-1) \frac{\hbar^2 \beta^2 \pi (Ze)^2 \rho}{6M} \right] \\ & - \frac{\pi (Ze)^2 \rho}{3} \int_0^\beta d\tau \left\langle \mathbf{r}_{12}^0 \left| \exp \left[ -(\beta - \tau) \left( -\frac{\hbar^2}{M} \Delta + \frac{Z^2 e^2}{r} \right) \right] \right. \right. \\ & \left. \left. \times r^2 \exp \left[ -\tau \left( -\frac{\hbar^2}{M} \Delta + \frac{Z^2 e^2}{r} \right) \right] \right| \mathbf{r}_{12}^0 \right\rangle \right\} \quad (23) \end{aligned}$$

Using (21) and (23) in (18), we find, to second order in  $\hbar$  and in the operator  $r$ ,

$$g(r^0) = \left[ 1 + \frac{\hbar^2 \beta^2 \pi (Ze)^2 \rho}{6M} \right] e^C \left( \frac{4\pi\beta\hbar^2}{M} \right)^{3/2} \times \left\langle \mathbf{r}^0 \left| \exp \left[ -\beta \left( -\frac{\hbar^2}{M} \Delta + \frac{Z^2 e^2}{r} + \frac{\pi Z^2 e^2 \rho}{3} r^2 \right) \right] \right| \mathbf{r}^0 \right\rangle \quad (24)$$

where  $C$  is defined by (12) from the classical pair correlation function. The calculation of  $g(r)$  is now reduced to a two-body problem, the evaluation of the matrix element in (24).

Let us note that, if we had taken for  $W$  the whole potential and had expanded it around  $(\mathbf{r}_1^0, \mathbf{r}_2^0, \mathbf{r}_3^0, \dots, \mathbf{r}_N^0)$ , we would have obtained the usual Wigner-Kirkwood expansion. The main departure from this approach has been to put the singular term  $(Ze)^2/r_{12}$  into  $H_0$ . Furthermore, since  $r_{12}^0$  is assumed to be small, we obtained a simplification by expanding  $W$  around  $(0, 0, \mathbf{r}_3^0, \dots, \mathbf{r}_N^0)$  rather than  $(\mathbf{r}_1^0, \mathbf{r}_2^0, \mathbf{r}_3^0, \dots, \mathbf{r}_N^0)$ , but this latter step is not an essential one.

#### 4. SEMICLASSICAL APPROXIMATION AND PATH INTEGRALS

We now turn to the evaluation of the matrix element in (24). The  $r^2$  part of the effective potential was obtained as a perturbation and is to be treated as such. Unfortunately, even in a pure Coulomb potential  $(Ze)^2/r$ , no simple explicit exact expression exists for the density matrix element that is needed here and we must resort to approximations.

Let us first study the zero-density limit, in which (24) reduces to

$$g_0(r^0) = \left( \frac{4\pi\beta\hbar^2}{M} \right)^{3/2} \left\langle \mathbf{r}^0 \left| \exp \left[ -\beta \left( -\frac{\hbar^2}{M} \Delta + \frac{Z^2 e^2}{r} \right) \right] \right| \mathbf{r}^0 \right\rangle \quad (25)$$

We are interested in the small- $\lambda$  case [here "small"  $\lambda$  means  $\lambda \ll \beta(Ze)^2$ , and it must be noted that this almost classical limit is reached for *low* temperatures]. The standard approach for calculating (25) is to use the WKB approximation. When  $r^0$  is small, the most important factor in  $g_0(r^0)$  is obtained by multiplying the probability  $\exp(-\beta v^2/M)$  that two nuclei have a relative velocity  $v$  by the Coulomb barrier WKB penetration factor  $\exp(-2\pi Z^2 e^2/\hbar v)$  and integrating that product over  $\mathbf{v}$ . If the temperature is low enough, the integrand has a sharp maximum, the Gamow peak, the value of which  $\exp[-(27\pi^2\beta Z^4 e^4 M/4\hbar^2)^{1/3}]$  is the dominating factor in  $g_0(r^0)$ . A more precise result can be obtained by using the WKB method three-dimensional extension.<sup>(17)</sup> An alternative equivalent procedure is to express (25) in terms of Coulomb wave functions and to make suitable approximations for these wave functions. Here, we shall use a third approach still equivalent to the

previous ones, based on path integrals (see, e.g., Ref. 18). This approach is especially convenient for treating the  $r^2$  perturbation term of (24). We shall first, however, consider the simpler case (25).

The path integral expression for the density in a pure Coulomb potential is

$$\begin{aligned} & \left\langle \mathbf{r}^0 \left| \exp \left[ -\beta \left( -\frac{\hbar^2}{M} \Delta + \frac{Z^2 e^2}{r} \right) \right] \right| \mathbf{r}^0 \right\rangle \\ &= \int \mathcal{D}\mathbf{r} \exp \left[ -\frac{1}{\hbar} \int_0^{\beta\hbar} dt \left( \frac{M}{4} \dot{\mathbf{r}}^2 + \frac{Z^2 e^2}{r} \right) \right] \end{aligned} \quad (26)$$

where the functional integral is to be taken on all paths  $\mathbf{r}(t)$  that go from  $\mathbf{r}^0$  to  $\mathbf{r}^0$  in a "time"  $\beta\hbar$ . The equivalent of the WKB approximation is to keep in (26) only the paths in the neighborhood of the one that minimizes the integral in the exponential; along that path, this integral is the action  $S(\mathbf{r}^0, \mathbf{r}^0; \beta\hbar)$  of a particle of mass  $M/2$  following a classical trajectory from  $\mathbf{r}^0$  back to  $\mathbf{r}^0$  in a time  $\beta\hbar$ , in the potential with the *reverse* sign  $-(Ze)^2/r$ . Taking also into account the contributions of the neighboring paths<sup>(19)</sup> gives the semiclassical approximation<sup>(20,21)</sup>

$$\begin{aligned} & \left\langle \mathbf{r}^0 \left| \exp \left[ -\beta \left( -\frac{\hbar^2}{M} \Delta + \frac{Z^2 e^2}{r} \right) \right] \right| \mathbf{r}^0 \right\rangle \\ &= (2\pi\hbar)^{-3/2} \left[ \text{Det} \left| \left( -\frac{\partial^2 S}{\partial r_{\alpha'} \partial r_{\beta''}} \right)_0 \right| \right]^{1/2} \exp \left[ -\frac{1}{\hbar} S(\mathbf{r}^0, \mathbf{r}^0; \beta\hbar) \right] \end{aligned} \quad (27)$$

where  $\text{Det} |(-\partial^2 S / \partial r_{\alpha'} \partial r_{\beta''})_0|$  is a  $3 \times 3$  determinant built with the second derivatives of  $S(\mathbf{r}', \mathbf{r}''; \beta\hbar)$  with respect to the Cartesian components  $r_{\alpha}'$  and  $r_{\beta}''$  ( $\alpha, \beta = 1, 2, 3$ ) at  $\mathbf{r}' = \mathbf{r}'' = \mathbf{r}^0$ .

The explicit evaluation of (27) is performed by computing the action along the appropriate ellipse (solution of Kepler's problem). The ellipse arc that gives the least action  $S(\mathbf{r}^0, \mathbf{r}^0; \beta\hbar)$  reduces to a radial line segment on which the particle goes outward away from  $\mathbf{r}^0$  and inward back to  $\mathbf{r}^0$ . A parametric representation for this path  $r(t)$ , using the auxiliary parameter  $\xi$ , is

$$t = (MA^3/2Z^2e^2)^{1/2}(\xi - \sin \xi), \quad r = A(1 - \cos \xi) \quad (28)$$

where  $2A$  is the aphelion value of  $r$ . Let  $\xi_0$  ( $0 < \xi_0 < \pi$ ) be the initial value of  $\xi$ , and  $2\pi - \xi_0$  its final value. The equations that determine  $\xi_0$  and  $A$  as functions of  $r^0$  and  $\beta\hbar$  are

$$\beta\hbar = (MA^3/2Z^2e^2)^{1/2}(2\pi - 2\xi_0 + 2 \sin \xi_0), \quad r^0 = A(1 - \cos \xi_0) \quad (29)$$

and the action is readily obtained in terms of  $\xi_0$  and  $A$  by using (28) in

$$S(\mathbf{r}^0, \mathbf{r}^0; \beta\hbar) = \int_0^{\beta\hbar} \left[ \frac{M}{4} \left( \frac{dr}{dt} \right)^2 + \frac{(Ze)^2}{r} \right] dt \quad (30)$$

[It may be of interest to note that, in the limit  $r^0 \rightarrow 0$ , the aphelion value of  $r$ , which is  $2A = (4\hbar^2\beta^2Z^2e^2/\pi^2M)^{1/3}$ , coincides with the turning point at the Gamow peak incident energy in the WKB approach.] The calculation of the second derivatives of  $S$  in (27) is more tedious, since we must consider true ellipses before going to the limit of a line segment. We omit the details and only quote the result from (25) and (27):

$$g_0(r^0) = (\pi - \xi_0 + \sin \xi_0)^{3/2}(\sin \xi_0)^{-3/2}[3(\pi - \xi_0) \sin \xi_0 + (1 - \cos \xi_0)(5 + \cos \xi_0)]^{-1/2} \times \exp[-(MZ^2e^2A/2\hbar^2)^{1/2}(3\pi - 3\xi_0 - \sin \xi_0)] \quad (31)$$

where  $\xi_0$  and  $A$  are defined by (29). More explicit expressions are obtained by expansions in the large- and small- $r^0$  limits. The large- $r$  limit (we now drop the superscript 0) is obtained for  $\pi - \xi_0 \ll 1$ . We then recover the classical result and the Wigner-Kirkwood correction to it<sup>(9)</sup>

$$g_0(r) = \exp\left[-\frac{\beta(Ze)^2}{r} + \frac{\hbar^2\beta^3(Ze)^4}{12Mr^4} + \dots\right] \quad \text{when } r \rightarrow \infty \quad (32)$$

The “small”- $r$  limit is obtained for  $\xi_0 \ll 1$ . This limit must be understood with some caution, since the quasiclassical approximation breaks down near the singularity of the Coulomb potential at those very small values of  $r$  that are of the order of the ionic Bohr radius  $\hbar^2/M(Ze)^2$  and these values of  $r$  must be excluded here. We find

$$g_0(r) = \frac{3^{1/2}(4\pi)^{1/3}}{12} \left[ \frac{(\hbar^2\beta^2Z^2e^2/M)^{1/3}}{r} + \dots \right] \times \exp\left[-\left(\frac{27\pi^2\beta Z^4e^4M}{4\hbar^2}\right)^{1/3} + 4\left(\frac{MZ^2e^2r}{\hbar^2}\right)^{1/2} + \dots\right] \quad (33)$$

when

$$\hbar^2/M(Ze)^2 \ll r \ll [\hbar^2\beta^2(Ze)^2/M]^{1/3}$$

We now turn to the evaluation of (24) with the  $r^2$  perturbation included. This additional potential makes two changes in the action: on the one hand, the path is changed, and on the other hand, the additional potential must be included in the action integrand. Since, however, the action is stationary under variations of the path, in first-order perturbation theory it is enough to take into account the second change only and thus to add to (30) a term

$$\begin{aligned} \delta S(\mathbf{r}^0, \mathbf{r}^0; \beta\hbar) &= \frac{\pi(Ze)^2\rho}{3} \int_0^{\beta\hbar} r^2 dt \\ &= \frac{\pi\rho}{3} \left[ \frac{M(Ze)^2}{2} \right]^{1/2} A^{7/2} \int_{\xi_0}^{2\pi - \xi_0} (1 - \cos \xi)^3 d\xi \end{aligned} \quad (34)$$

where the integral has been computed by using for  $r(t)$  the unperturbed path (28). The parameters  $A$  and  $\xi_0$  are still given by (29). A perturbation term must also be added to the second derivatives of the action. Using again (27) with the addition of  $\pi(Ze)^2\rho r^2/3$  in the potential, we finally obtain for (24), in the small- $r$  limit,

$$g(r) = \left[ 1 - \left( \frac{35}{18\pi} - \frac{\pi}{6} \right) \frac{\hbar^2\beta^2(Ze)^2\rho}{M} \right] \times \exp \left[ C - \frac{5}{12} \left( \frac{2}{\pi} \right)^{1/3} (\beta Z^2 e^2)^{7/3} \left( \frac{\hbar^2}{MZ^2 e^2} \right)^{2/3} \rho \right] g_0(r) \quad (35)$$

when

$$\hbar^2/M(Ze)^2 \ll r \ll [\hbar^2\beta^2(Ze)^2/M]^{1/3}$$

where  $C$  is given by (17) and  $g_0(r)$  by (33).

Since the term of order  $\hbar^{4/3}$  in the exponential of (35) comes from  $\delta S$ , i.e., from the  $r^2$  term that has been treated as a perturbation in (23), a condition of validity of (35) is

$$(5/12)(2/\pi)^{1/3}(\beta Z^2 e^2)^{7/3}(\hbar^2/MZ^2 e^2)^{2/3}\rho \ll 1$$

or equivalently  $0.025\Gamma^{5/3}(\lambda/a)^{4/3} \ll 1$  (36)

(36) must be considered as a more precise form of our assumption that  $\lambda/a$  should be “small.” Similarly, the term of order  $\hbar^2$  in the first bracket of (35) must be small compared to 1; this condition, however, is automatically satisfied as a consequence of (36) and of our earlier assumption  $\Gamma > 1$ .

If we omit these corrections of order  $\hbar^{4/3}$  and  $\hbar^2$ , (35) reduces to a simpler form, which had been previously assumed on heuristic grounds<sup>(2,4)</sup>:

$$g(r) = e^C g_0(r) \quad (37)$$

where  $C$  is still defined by (12) from the classical pair correlation function and where  $g_0(r)$  is still the dilute plasma quantum pair correlation function. This approximate result (37) is the solution of the quantum mechanical two-body problem for a pair of particles interacting through the truncated classical potential of mean force  $(Z^2 e^2/r) - (C/\beta)$ . In the present paper, (37) appears as the zeroth-order result in a systematic expansion method, the next step of which gives (24) and (35). Within that next order of approximation, it is still valid to consider that particles 1 and 2 interact through the classical potential of mean force, in which, however, we now keep one more term  $\pi Z^2 e^2 \rho r^2/3$  [and there is also a further correction of order  $\hbar^2$  in the first bracket of (24)]. Yet, it must be pointed out that in higher orders of approximation it will no longer be possible to reduce the many-body problem to a two-body tunneling through some effective potential; it is likely that the fluctuations of the potential will have to be taken into account.

## 5. EXCHANGE EFFECTS

Here we try to justify the neglect of exchange effects in the previous sections. We only consider the two-body problem in a pure Coulomb potential. The exchange contribution to  $g(r^0)$  is dominated by

$$\exp[-\hbar^{-1}S(\mathbf{r}^0, -\mathbf{r}^0; \beta\hbar)]$$

Now the action  $S$  must be computed along an ellipse arc which goes from  $\mathbf{r}^0$  to  $-\mathbf{r}^0$  in a time  $\beta\hbar$ ; the major axis of the ellipse, which is perpendicular to  $\mathbf{r}^0$ , will be taken as the  $x$  axis. A parametric representation of the path in Cartesian coordinates  $\mathbf{r} = (x, y)$  is

$$t = (MA^3/2Z^2e^2)^{1/2}(\xi - \epsilon \sin \xi), \quad x = A(\cos \xi - \epsilon), \quad y = A(1 - \epsilon^2)^{1/2} \sin \xi \quad (38)$$

where  $\epsilon$  is the ellipse eccentricity. The endpoints of the path are parametrized by  $\xi_0$  and  $2\pi - \xi_0$ , and therefore the equations that determine  $\xi_0$ ,  $A$ , and  $\epsilon$  are

$$\begin{aligned} \beta\hbar &= (MA^3/2Z^2e^2)^{1/2}(2\pi - 2\xi_0 + 2\epsilon \sin \xi_0) \\ 0 &= A(\cos \xi_0 - \epsilon), \quad r^0 = A(1 - \epsilon^2)^{1/2} \sin \xi_0 \end{aligned} \quad (39)$$

The action is easily found to be

$$S(\mathbf{r}^0, -\mathbf{r}^0; \beta\hbar) = (MAZ^2e^2/2)^{1/2}(3\pi - 3\xi_0 - \epsilon \sin \xi_0) \quad (40)$$

In the small- $r^0$  limit, one obtains from (38) and (39)

$$\begin{aligned} \exp[-\hbar^{-1}S(\mathbf{r}, -\mathbf{r}; \beta\hbar)] &= \exp[-(27\pi^2\beta Z^4e^4M/4\hbar^2)^{1/3} \\ &\quad + 4(MZ^2e^2r/2\hbar^2)^{1/2} + \dots] \end{aligned} \quad (41)$$

when

$$\hbar^2/M(Ze)^2 \ll r \ll [\hbar^2\beta^2(Ze)^2/M]^{1/3}$$

A comparison of (41) with the corresponding exponential in the direct term (33) shows that the coefficient of the large term  $[M(Ze)^2r/\hbar^2]^{1/2}$  is  $\sqrt{2}$  times larger in the direct term than in the exchange term. Therefore, the exchange exponential (41) can be safely neglected when compared to the direct exponential (33).

## 6. PYCNONUCLEAR REACTION RATE

In a stellar medium, nuclear reactions will occur when two nuclei touch one another. The number of reactions per unit volume and unit time is expected to be proportional to  $\rho^2g(r)$ , where  $r$  is now the nuclear diameter. The reaction rate is said to be enhanced by a factor  $g(r)/g_0(r)$ , where  $g_0(r)$  is the dilute plasma pair correlation function. This factor can be considered

as describing the screening of the Coulomb barrier between two nuclei by the other particles. If the medium is dense enough for the enhancement factor to be large, nuclear reactions may occur at a fairly low temperature; these reactions, which result from high density rather than high temperature, are termed pycnonuclear.

In the present paper, we have confirmed that, in lowest order of approximation, the enhancement factor is  $\exp C$ ; we give a numerical expression for  $C$  in (17). We have also computed corrections to this lowest order result, obtaining the enhancement factor  $g(r)/g_0(r)$  as given in (35). Unfortunately, our derivation is valid only if these corrections are small. Yet, the evaluation of these corrections has provided us with a condition (36) for the validity of the approximations. Furthermore, we may note that the first corrections to the simple formula  $\exp C$  tend to make the enhancement factor smaller.

As a numerical example, let us consider a stellar plasma of pure  $C^{12}$ , at a temperature  $10^8$  K and a density  $10^8$  g/cm<sup>3</sup>. Then,  $\lambda = 5 \times 10^{-12}$  cm,  $a = 3.6 \times 10^{-11}$  cm,  $\Gamma = 16.6$ ;  $0.025\Gamma^{5/3}(\lambda/a)^{4/3} = 0.19$  and condition (36) is reasonably satisfied. The nuclear diameter is in the range required in (35), since

$$\begin{aligned} \hbar^2/M(Ze)^2 &= 6.7 \times 10^{-15} \text{ cm} \ll r = 5.5 \times 10^{-13} \text{ cm} \\ &\ll [\hbar^2\beta^2(Ze)^2/M]^{1/3} = 1.3 \times 10^{-11} \text{ cm}. \end{aligned}$$

We then find, from (17),  $C = 18.2$ , from the simplified formula (37) an enhancement factor  $\exp C = 8 \times 10^7$ , and from the more complete formula (35) a corrected enhancement factor  $6.6 \times 10^7$  (practically, this slight correction comes only from the term of order  $\hbar^{4/3}$ ; the correction of order  $\hbar^2$  is entirely negligible).

In two recent papers<sup>(22,23)</sup> about the nuclear reaction rate enhancement problem, approximations have been used that differ from ours; we believe our method of approximation to be more systematic.

## ACKNOWLEDGMENTS

The author is indebted to E. Schatzman (who did pioneering work<sup>(24)</sup> in this field) for having introduced him to the problem of pycnonuclear reactions, and to J. P. Hansen and A. Krzywicki for stimulating discussions.

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