Correlation Function in a Plasma at Zero Particle Separation

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We derive the radial distribution functions at zero particle separation for like and unlike particles in a plasma. No account is taken of many-body (screening) effects, but the sum over Coulomb wave functions in the two-particle density matrix is evaluated exactly to give a convergent power series in the dimensionless parameter $\gamma^{1/2}$, where $\gamma=2\mu e^4/\hbar^2kT$, and μ is the reduced mass of the two-particle system.

The singularity that occurs for small particle separation in a classical calculation of the radial distribution function (r.d.f.) in a plasma can only be removed by taking quantum effects into account. Feix,[1] Trubnikov and Elesin,[2] and Diesendorf and Ninham[3] have obtained the first two terms for small values of r and γ: For $r=0$ their result is

$$g(0)\sim 1-(\pi\gamma)^{1/2}. \tag{1}$$

In this paper we determine $g(0)$ under the assumption that at small separations the particles interact via a purely Coulomb potential, without any indirect effects due to the presence of the other particles in the system. Within this assumption the function $g(r)$ can be expressed in terms of the one- and two-particle density matrices using the relations

$$g(|\mathbf{x}-\mathbf{y}|)=\rho_2(\mathbf{x},\mathbf{y},\mathbf{x},\mathbf{y},\beta)/\rho_1(\mathbf{x},\mathbf{x},\beta)\rho_1(\mathbf{y},\mathbf{y},\beta) \tag{2}$$

for distinguishable particles, and

$$g(|\mathbf{x}-\mathbf{y}|)=[\rho_2(\mathbf{x},\mathbf{y},\mathbf{x},\mathbf{y},\beta)-\tfrac{1}{2}\rho_2(\mathbf{x},\mathbf{y},\mathbf{y},\mathbf{x},\beta)]/\rho_1(\mathbf{x},\mathbf{x},\beta)\rho_1(\mathbf{y},\mathbf{y},\beta) \tag{3}$$

for indistinguishable particles. In the latter expression we have taken account of spin and exchange effects explicitly, so that ρ_2 must be calculated using wave functions for distinguishable particles. It is well known[4] that the density matrix can be expanded as

$$\rho_2(\mathbf{x}_1,\mathbf{y}_1,\mathbf{x}_2,\mathbf{y}_2,\beta)=\sum_i \exp(-\beta E_i)\psi_i^*(\mathbf{x}_1,\mathbf{y}_1)\psi_i(\mathbf{x}_2,\mathbf{y}_2), \tag{4}$$

where the wave functions are the complete set of bound and scattering states including center-of-mass motion. Note that we use Coulomb units[5] throughout, so that the unit of energy is $\mu e^4/\hbar^2$, where μ is the reduced mass of the two-particle system. We absorb this constant into Eq. (4) by introducing the parameter $\gamma=2\mu e^4/\hbar^2kT$ as the measure of temperature. Eliminating the center-of-mass factors in Eq. (4) and putting the inter-particle separation equal to zero, we obtain for $g(0)$

$$g(0)=(\pi\gamma)^{3/2}\sum_i e^{-\beta E_i}|\psi_i(0)|^2, \tag{5}$$

where $\psi_i(r)$ are the Coulomb wave functions for the relative motion of the two particles. The values of $|\psi_i(0)|^2$ are given in Ref. 5, and direct use of these results in Eq. (5) yields the formulas

$$g_l(0)=2\pi^{1/2}\gamma^{3/2}\int_0^\infty \frac{e^{-\gamma k^2}kdk}{\exp(\pi/k)-1} \tag{6}$$

for like particles, and

$$g_u(0)=4\pi^{1/2}\gamma^{3/2}\int_0^\infty \frac{e^{-\gamma k^2}kdk}{1-e^{-\pi/k}}+4(\pi\gamma)^{3/2}\sum_{n=1}^{\infty}\frac{\exp(\gamma/4n^2)}{n^3} \tag{7}$$

for unlike particles.

We now proceed to develop the complete ascending expansions for these expressions, using the technique of Mellin transforms. Turning first to Eq. (6), we write

$$\begin{aligned} g_l(0)&=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\gamma^{-p}dp\int_0^\infty \gamma^{p-1}d\gamma \times\left\{2\pi^{1/2}\gamma^{3/2}\int_0^\infty\frac{e^{-\gamma k^2}kdk}{e^{\pi/k}-1}\right\}\\ &=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\gamma^{-p}dp\int_0^\infty\frac{2\pi^{1/2}\Gamma(p+\frac{3}{2})k^{-2p-2}dk}{e^{\pi/k}-1}. \end{aligned} \tag{8}$$

Changing variables in this last integral to $x=\pi/k$ gives the further simplification

$$g_l(0)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}2\gamma^{-p}\pi^{-2p-1/2}\times\Gamma(p+\tfrac{3}{2})\Gamma(2p+1)\zeta(2p+1)dp \tag{9}$$

at which stage we can close the contour to the left and obtain the complete ascending expansion for $g_l(0)$ from the residues at the poles of the integrand. Examination of the steps leading up to Eq. (9) shows that we must take $c>0$. A considerable further simplification can be made by using several standard functional equations

[1] M. Feix, in *Proceedings of the Sixth International Conference on Ionization Phenomena in Gases, Paris, 1963* (SERMA, Paris, 1964), Vol. II, pp. 185–187.
[2] B. A. Trubnikov and V. F. Elesin, Zh. Eksperim. i Teor. Fiz. 47, 1279 (1964) [English transl.: Soviet Phys.—JETP 20, 866 (1965)].
[3] M. Diesendorf and B. W. Ninham (to be published).
[4] B. Kahn and G. E. Uhlenbeck, Physica 5, 399 (1938).
[5] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon Press, Inc., New York, 1959).

for the Γ and ζ functions,[6] to achieve the final result:

$$2g_l(0)=1-(\pi\gamma)^{1/2}+\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}(\tfrac{1}{2}n)!\zeta(n+2)\gamma^{n/2+1}. \quad (10)$$

We note that this is not just an asymptotic expansion for small γ, it is in fact convergent for all values of γ.

We deal with the expansion of $g_u(0)$ in a similar way. The integral in Eq. (7) can be rearranged to give

$$2\pi^{1/2}\gamma^{1/2}+2g_l(0), \quad (11)$$

and we evaluate the sum in Eq. (7) by expanding the exponential and changing the order of summation:

$$\sum_{n=1}^{\infty}\frac{e^{\gamma/4n^2}}{n^3}=\sum_{n=1}^{\infty}\sum_{m=0}^{\infty}\frac{\gamma^m}{m!4^m n^{2m+3}}=\sum_{m=0}^{\infty}\frac{\gamma^m\zeta(2m+3)}{4^m m!}. \quad (12)$$

The complete expansion for $g_u(0)$ can now be found by collecting together Eqs. (10)–(12). The first few terms are

$$g_u(0)\approx 1+(\pi\gamma)^{1/2}+\zeta(2)\gamma+(4\pi-\tfrac{1}{2})\zeta(3)\pi^{1/2}\gamma^{3/2}. \quad (13)$$

For large values of γ, these expansions are of no practical use. The Mellin technique does not give a descending expansion, as is evidenced by the lack of poles in the right-hand half-plane in Eq. (9). We therefore estimate

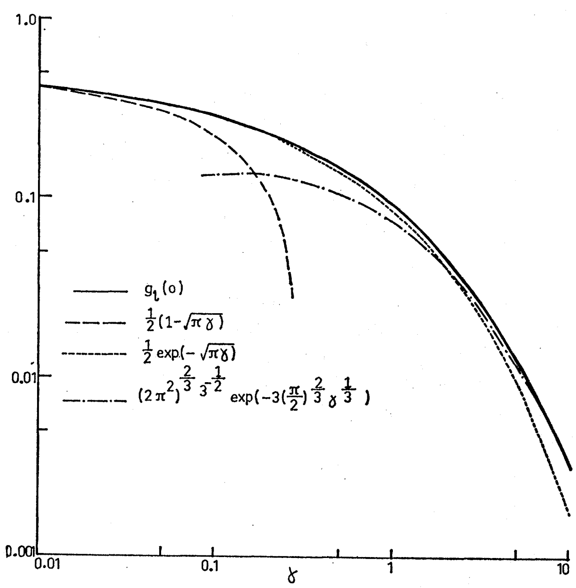

FIG. 1. $g_l(0)$ compared with the high- and low-temperature approximations and $e^{-\surd(\pi\gamma)}$. For the electron-electron r.d.f. $T=3.158\times10^5/\gamma$ °K and for the proton-proton r.d.f. $T=1.151\times10^9/\gamma$ °K.

[6] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, New York, 1952).

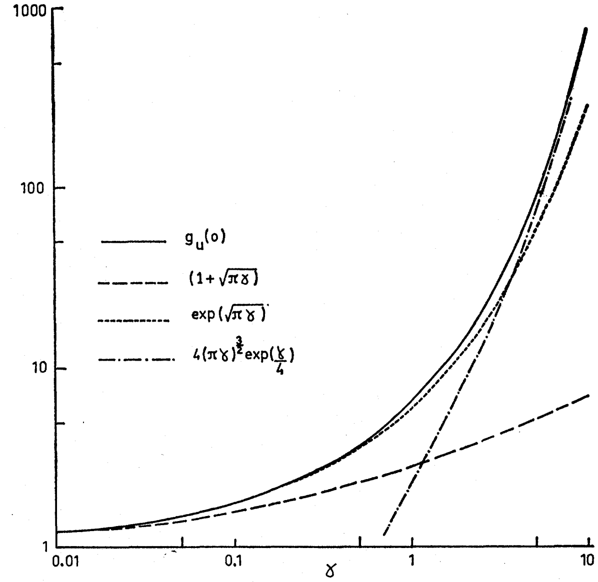

FIG. 2. $g_u(0)$ compared with the high- and low-temperature approximations and $e^{\surd(\pi\gamma)}$. For the proton-electron r.d.f. $T=6.314\times10^5/\gamma$ °K.

$g_l(0)$ for large γ by steepest descents. We expand the factor $(e^{\pi/k}-1)^{-1}$ as a series in $e^{-n\pi/k}$, change variables to $u=k^2$, and then approximate the exponent in each of the integrals by $-3\{\gamma u_n+(\frac{1}{8}n\pi)(u-u_n)^2/u_n^{5/2}\}$ where $u_n=(n\pi/2\gamma)^{2/3}$, to obtain

$$g_l(0)\approx\pi^{1/2}\gamma^{3/2}\sum_{n=1}^{\infty}\left(\frac{8u_n^{5/2}}{3n}\right)^{1/2}\exp(-3\gamma u_n)$$

$$\approx\pi^{1/2}\gamma^{3/2}\left(\frac{8}{3}\right)^{1/2}u_1^{5/4}\exp(-3\gamma u_1), \quad \gamma\gg1. \quad (14)$$

For $g_u(0)$, Eqs. (11) and (14) show that the sum dominates for large γ. We therefore write

$$g_u(0)\approx 4(\pi\gamma)^{3/2}\exp(\tfrac{1}{4}\gamma), \quad \gamma\gg1. \quad (15)$$

We present graphically a comparison between the various formulas given above and the exact (numerically evaluated) values of $g(0)$. For $g_l(0)$ we plot in Fig. 1 the exact result, the first few terms of the series, and Eq. (14). We also show the function $e^{-\surd(\pi\gamma)}$: This is a conjecture by DeWitt[7] which turns out to be quite good provided absolute and not relative errors are the important criterion. For $g_u(0)$, we plot in Fig. 2 the exact result, the first few terms of the series, Eq. (15), and the function $e^{\surd(\pi\gamma)}$.

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[7] H. DeWitt (private communication).