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Convergence of the Two-Component Plasma Correlation Function

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It has been suggested that the divergence of the two-component plasma correlation function at small interparticle distances may be removed by taking quantum corrections to the classical result in a certain manner. It is shown here that this approach is not possible in general. A completely quantum-mechanical treatment is given instead, and an explicit convergent expression for the radial distribution function at small r is obtained. Also discussed is the fact that there does not seem to exist any simple interpolation formula that bridges the classical and the quantum-mechanical results for r in the region of thermal de Broglie wavelengths.

I. INTRODUCTION

It is well known that the classical correlation function of a two-component plasma has a singularity at small interparticle distances. As we shall see below, the radial distribution function consists of two terms, one representing the contribution from the bound states and the other from the continuum states. Classically both terms are divergent at small r . While the contribution from the continuum states diverges more strongly at lower energies, the most serious difficulty comes from the bound states.

A suggestion has been made by Lamb¹ that if one takes the quantum-mechanical correction, one can obtain a radial-distribution function which appears to be finite everywhere. The method he used was developed by Goldberger and Adams.² It was essentially a generalization of Wigner's method³ of power-series expansion in \hbar . The question of whether this method can be applied to resolve the divergence difficulty in this problem needs more careful consideration. In fact, as is well known,³ the expansion in a power series in \hbar is valid only when the behavior of the system is nearly correctly given by the classical theory. In the present case of a two-component plasma with Coulomb interaction, this expansion is actually a power series in the spatial derivatives of the interaction potential as well as in \hbar , and is clear-

ly inapplicable as the interparticle distance r approaches zero. The result obtained by Lamb may be valid for r much greater than the thermal de Broglie wavelength $\lambda = (\hbar^2/2mkT)^{1/2}$, in which case the classical theory is a good approximation anyway. However, his result cannot be used to discuss the divergence difficulty at $r < \lambda$ where the expansion breaks down.

On the other hand, Trubnikov and Elesin⁴ have calculated the radial distribution function quantum-mechanically. However, they neglected the bound states completely and calculated the continuum contribution by making a large ka_0 or high-energy expansion (Born approximation). We would like to point out that their results cannot be justified unless the fundamental divergence difficulty arising from the bound states is first resolved.

It is the purpose of this paper to analyze the behavior of the radial distribution function at distances $r < \lambda$ by including contributions from all the bound and continuum states. It will be shown explicitly by a completely quantum-mechanical treatment that there is no divergence as $r \rightarrow 0$.

In Sec. II we review briefly the expansion method and point out its inapplicability to the present problem. Section III is devoted to the calculation of the radial distribution function at $r < \lambda$. Discussions of these results are presented in Sec. IV.

II. REVIEW OF EXPANSION METHOD

For the short-range particle correlations of a two-component plasma, we may ignore the many-body collective effect and consider only a two-particle Wigner distribution function; i. e., we may ignore the influence of other particles on the two particles whose correlation at small r is being considered.¹ On integrating the Wigner distribution function over the total momentum of the two-particle system, we obtain the radial distribution function which takes the familiar form

$$n(r) = \sum_{\nu} \psi_{\nu}^*(\vec{r}) e^{-\beta H} \psi_{\nu}(\vec{r}), \quad (1)$$

where r is the relative-position vector of the two particles, $\beta = 1/kT$, and H and $\psi_{\nu}(\vec{r})$ are, respectively, the energy operator and any complete set of wave functions for the two-particle system. As shown by Goldberger and Adams,² if we choose $\psi_{\nu}(\vec{r})$ to be the plane wave states $\psi_{\vec{p}}(\vec{r})$, Eq. (1) can be rewritten as

$$n(r) = (2\pi)^{-3} \int d^3 p \psi_{\vec{p}}^*(\vec{r}) e^{-\lambda^2 \vec{\nabla}^2 + U} \psi_{\vec{p}}(\vec{r}), \quad (2)$$

where \vec{p} is the relative particle momentum measured in units of $(2mkT)^{1/2}$ and $U(\vec{r}) = \beta V(\vec{r})$, $V(\vec{r})$ being the interaction potential. By commuting $\psi_{\vec{p}}$ to the left, Eq. (2) can be further reduced to

$$\begin{aligned} n(r) &= (2\pi)^{-3} \int d^3 p e^{-p^2} \exp[\lambda^2 \vec{\nabla}^2 + 2i\lambda \vec{p} \cdot \vec{\nabla} - U(\vec{r})] \\ &= \pi^{-3/2} \int d^3 p e^{-p^2} \exp[-\mathcal{U}(\vec{r} + 2i\lambda \vec{p}, 1)] v_1(1), \quad (3) \end{aligned}$$

which is convenient for expanding into a power series in λ^2 . In Eq. (3), the function $\mathcal{U}(\vec{r}, s)$ is defined by

$$s\mathcal{U}(\vec{r}, s) \equiv \int_0^s ds_1 U(\vec{r} - 2i\lambda \vec{p} s_1), \quad (4)$$

and $v_1(s)$ satisfies the differential equation

$$\begin{aligned} \partial v_1(s) / \partial s &= [\lambda^2 \vec{\nabla}^2 - 2s\lambda^2 (\vec{\nabla} \cdot \vec{\nabla}) \\ &\quad - s\lambda^2 \nabla^2 \mathcal{U} + s^2 \lambda^2 (\vec{\nabla} \mathcal{U})^2] v_1(s) \quad (5) \end{aligned}$$

with the boundary condition $v_1(0) = 1$.

At this point, Lamb¹ simply approximates $v_1(1)$ by unity.⁵ Then, with $U(\vec{r}) = \beta e_1 e_2 / r$, the radial distribution function becomes

$$n(r) = -2\pi^{-\frac{1}{2}} \int_0^{\infty} p^2 dp e^{-p^2} i\alpha \int_{z^*}^z dt \left(\frac{t+z}{t+z^*} \right)^{i\nu}, \quad (6)$$

where $z = 1 + i\alpha$, $\nu = l/2\lambda p$, $l = e_1 e_2 / kT$, and $\alpha = 2\lambda p / r$. We can now easily show by a change of the variable $t = 1 + i\alpha y$ that the integral in Eq. (6) reduces to

$$\begin{aligned} I &\equiv -i\alpha \int_{z^*}^z dt [(t+z)/(t+z^*)]^{i\nu} \\ &= 2 \int_0^1 dy e^{-\nu\theta} [\cos(\nu l A) - \alpha y \sin(\nu l A)], \quad (7) \end{aligned}$$

where $A(y) \equiv \{ [4 + \alpha^2(y+1)^2] / [4 + \alpha^2(y-1)^2] \}^{1/2}$

and $\theta(y) \equiv \tan^{-1} \{ 4\alpha / [4 + \alpha^2(y^2-1)] \}$.

It is obvious that as $r \rightarrow 0 (r/\lambda \ll 1)$ or $\alpha \rightarrow \infty$, the integral I is divergent (see Appendix). This shows that the finite result obtained by Lamb after several mathematical approximations definitely cannot be extended to the range $r < \lambda$. His result is, therefore, irrelevant as far as the divergence difficulty is concerned. As a matter of fact, an explicit form of $n(r)$ for a general potential $V(r)$ has been given to order λ^2 as^{2,3}

$$n(r) = n^{cl}(r) \{ 1 - \lambda^2 [\frac{1}{6} \nabla^2 U - \frac{1}{12} (\vec{\nabla} U)^2] \} + O(\lambda^4), \quad (8)$$

where $n^{cl}(r)$ is the classical radial distribution function. This expression clearly indicates that it is an expansion in both λ and the derivatives of U . Therefore, it will become invalid at small r for Coulomb interaction.

III. CALCULATION OF $n(r)$ FOR SMALL r

To evaluate $n(r)$ quantum mechanically it is more convenient to use the complete set of energy eigenfunctions of the hydrogen atom. We can rewrite Eq. (1) as

$$n(r) = n_d(r) + n_c(r), \quad (9)$$

where, apart from a statistical normalization constant,

$$n_d(r) = \sum_{n=1}^{\infty} e^{-\beta E_n} \sum_{lm} \psi_{nlm}^*(\vec{r}) \psi_{nlm}(\vec{r}) \quad (10)$$

is the contribution from the discrete bound states, and

$$n_c(\vec{r}) = \int_0^{\infty} dE_k e^{-\beta E_k} \sum_{lm} \psi_{klm}^*(\vec{r}) \psi_{klm}(\vec{r}) \quad (11)$$

is the contribution from the states in the continuum. Since we are only interested in small r , we have to take only the $l=0$ term in the sums of Eqs. (10) and (11) so that only the radial wave functions enter.

To evaluate $n_d(r)$ we take

$$R_{n0}(r) = \sqrt{\frac{1}{2}} \left(\frac{2}{na_0} \right)^{\frac{3}{2}} e^{-r/na_0} F(-n+1, 2, \frac{2r}{na_0}) \quad (12)$$

where $a_0 = \hbar^2 / me^2$ is the Bohr radius and $F(a, b, x)$ is the hypergeometric function which, for small x , takes the form

$$F(a, b, x) = 1 + \frac{a}{b} \frac{x}{1!} + \frac{a(a+1)}{b(b+1)} \frac{x^2}{2!} + \dots \quad (13)$$

On substituting Eq. (12) into Eq. (10) we obtain readily, for $r < a_0$,

$$n_d(r) = \sum_{n=1}^{\infty} e^{-\beta E_n} |R_{n0}(r)|^2$$

$$= \frac{1}{2} \left(\frac{2}{a_0} \right)^3 \sum_{n=1}^{\infty} e^{2\lambda^2/a_0^2 n^2} n^{-3} e^{-2r/a_0 n}. \quad (14)$$

It is now clear from Eq. (14) that $n_d(r)$ is convergent for arbitrarily small r . As $r \rightarrow 0$, we have

$$n_d(0) \sim e^{2\lambda^2/a_0^2} \sum_{n=1}^{\infty} n^{-3} e^{-2\lambda^2/a_0^2 (1-n^{-2})}, \quad (15)$$

which always converges faster for any temperature than the product of $\exp(2\lambda^2/a_0^2)$ and the ζ function $\zeta(3) = \sum_{n=1}^{\infty} 1/n^3$. It is interesting to note that the temperature has no essential effect on the convergence as far as the bound-state contributions are concerned.

For the evaluation of $n_c(r)$ we need the continuum s -wave radial eigenfunctions⁶

$$R_{k0}(r) = 2\sqrt{k} [a_0(1 - e^{-2\pi/k a_0})]^{-\frac{1}{2}} e^{-ikr} \times F((i/ka_0) + 1, 2, 2ikr), \quad (16)$$

where $k = (2mE_k/\hbar^2)^{1/2}$. Substituting Eq. (16) into Eq. (11), we obtain

$$n_c(r) = 4 \int_0^{\infty} dk [k e^{-\beta E k/a_0} (1 - e^{-2\pi/k a_0})] \times |F((i/ka_0) + 1, 2, 2ikr)|^2. \quad (17)$$

Although the above integral involves the entire range of k , the existence of the exponential damping factor effectively cuts it off at an upper limit $k_{\max} \sim 1/\lambda$. Therefore, for $r < \lambda$ and $r < a_0$, we can expand the hypergeometric function to obtain, up to first order in r ,

$$n_c(r) \approx \left(1 - \frac{2r}{a_0}\right) \frac{4}{a_0} \int_0^{\infty} k dk \frac{e^{-\lambda^2 k^2}}{1 - e^{-2\pi/k a_0}}. \quad (18)$$

Although the integral in Eq. (18) cannot be evaluated analytically, it is clearly convergent for any finite λ . For $\lambda = 0$ or $\beta = 0$, one can no longer use Eq. (18) which is a result of the $r/\lambda < 1$ expansion. However, by examining directly Eq. (17), $n_c(r)$ then becomes essentially the k -scale normalization integral⁶ which is, of course, finite.

IV. DISCUSSIONS AND CONCLUSIONS

It might be thought that it is the discrete nature of the bound states in quantum mechanics that removes the divergence of $n(r)$ at small r . We would like to point out, however, that classically $n(r)$ takes the form

$$n^{cl}(r) \sim \int_0^{\infty} p^2 dp \exp \left[-\beta \left(\frac{p^2}{2m} - \frac{e^2}{r} \right) \right] = \int_{-e^2/r}^0 dE e^{-\beta E} \left(\frac{e^2}{r} + E \right)^{\frac{1}{2}} + \int_0^{\infty} dE e^{-\beta E} \times \left(\frac{e^2}{r} + E \right)^{\frac{1}{2}} = n_d^{cl}(r) + n_c^{cl}(r), \quad (19)$$

where both terms n_d^{cl} and n_c^{cl} diverge when r approaches zero.⁷

Furthermore, as we have noted in the previous section, Eqs. (15) and (18) are valid only in the region $r < a_0, \lambda$ since we have made use of the small r expansion of the wave function. The classical limit Eq. (19) applies when $r > (\lambda^4/a_0)^{1/3}$ as can be seen readily from Eq. (8). But there does not seem to be any simple interpolation formula for the region $r \lesssim (\lambda^4/a_0)^{1/3}$.

Finally, it can also be pointed out that in electric conductivity calculations for a two-component plasma, there exists a related divergence difficulty in the classical expression arising from collisions with large momentum transfers q . It has been claimed that this difficulty is already resolved by taking the so-called semiclassical limit⁸ of the quantum-mechanical result. The limiting procedure consists in retaining an exponential factor $\exp(-\lambda^2 q^2/4)$ in the quantum-mechanical plasma dispersion function $Q(q, \omega)$, while the other factors are expanded in powers of λq . However, this limiting procedure is actually valid only for $q \ll 1/\lambda$, in which case one should, to be consistent, approximate the above exponential damping factor by $1 - \lambda^2 q^2/4$ as well. Therefore, the divergence still remains for large q even in the semiclassical limit.

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APPENDIX

Consider the second part of the integral in (7)

$$I_2(\alpha) = -2\alpha \int_0^1 dy e^{-\nu\theta} y \sin(\nu \ln A)$$

as a function of $\alpha = 2\lambda p/r$. In the limit of small r , i. e., large α , for values of y from 0 up to $1 - \Delta$, where $\Delta \geq O(1/\alpha)$, we have

$$-\theta \approx 1/\alpha,$$

and $A \sim (1+y)/(1-y)$;

and for y from $\sim (1-\Delta)$ to 1, we have

$$-\theta \approx \frac{1}{2}\pi,$$

$$A \approx \sqrt{1 + \alpha^2} \approx \alpha,$$

$$\text{and } I_2(\alpha) \approx -2\alpha \int_0^{1-\Delta} dy y \sin(\nu \ln A) \\ - 2\alpha \int_{1-\Delta}^1 dy e^{\pi\nu/2} y \sin(\nu \ln A).$$

The second part is finite, but the first part diverges as $\alpha \propto (1/r) \rightarrow \infty$.

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⁵Actually both the exponential factor and $v_1(1)$ in the second line of Eq. (3) can be developed into a power series in λ . To order λ^2 , $v_1(1) = 1 - \lambda^2 [\frac{1}{2}\nabla^2 U + \frac{1}{3}(\nabla U)^2]$. It is inconsistent to replace $v_1(1)$ by unity, its zeroth-order value, while keeping all higher-order λ terms in the exponential factor.

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Measurements of the Stark Broadening of Two Neutral Helium Lines in a Plasma*

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A detailed study has been made of the broadening of the lines $\lambda 3889 \text{ \AA}$ (width only) and $\lambda 5016 \text{ \AA}$ (shift and width) of neutral helium in the plasma produced in an electromagnetically driven T tube operating in helium-hydrogen gas mixtures. The electron density in the plasma was found from the broadening of H_β , while the temperature was determined from the ratio of the intensity of H_β to that of the underlying continuum. Temperatures were in the range 20 000–30 000°K; electron densities varied from 10^{16} to $6 \times 10^{17} \text{ cm}^{-3}$. The broadening of the line $\lambda 3889 \text{ \AA}$ was found to increase linearly with electron density; and it compared well with calculations based on the generalized impact theory, except for (constant) correction factors ranging from about 0.9 to 1.0 (depending on which of the various calculations is referred to). For the line $\lambda 5016 \text{ \AA}$, neither of the previous calculations, nor a correction discussed here, predicts either the width or the shift variations satisfactorily; all the calculations give significantly wider lines above electron densities of 10^{17} cm^{-3} than are found experimentally. Also, as the electron density increases, the calculated shifts all become increasingly larger than those found experimentally. However, at the low densities most deviations are small ($\lesssim 20\%$).

INTRODUCTION

The Stark broadening of spectral lines by electrons and ions is a convenient and tried method of measuring the electron density in a plasma. This is particularly so for the hydrogen line H_β where the experimental ease of measuring only relative intensities in the visible spectrum is coupled with the existence of profile calculations that were estimated to be reliable to within $\pm 15\%$.^{1,2} Detailed comparisons³ between theory and experiment⁴ have since shown that these calculations may be reliable within $\pm 4\%$, at an electron density of $2 \times 10^{17} \text{ cm}^{-3}$; and the most recent experimental results⁵ indicate that the absolute accuracy of the H_β calculations is $\pm 3.5\%$ in the range ($2 \leq N_e \leq 8$) $\times 10^{16} \text{ cm}^{-3}$, all these errors being expressed in terms of H_β widths.

By comparison, the estimated accuracy of the first calculations of the broadening and shift of the lines of neutral helium⁶ was only a little worse, being $\pm 20\%$ of the widths. Early experimental results⁷ indicated that these calculations were at

least as good as expected, but more recently^{8,9} it has been suggested that the experimental results justify an empirical correction, namely that, on the average, the electron density calculated from the width of any neutral helium line should be increased by 10% to obtain the true value. In connection with such corrections there is considerable interest in improved calculations^{10,11} of the broadening and shift of neutral helium lines, and there is a need for a more thorough experimental study. At the same time, the neutral helium lines, especially the strong ones like $\lambda 3889 \text{ \AA}$, would be very useful as electron-density monitors. The line H_β is undoubtedly the best monitor for hydrogen and deuterium plasmas, and even for mixtures of hydrogen and helium; but if any other element is to be studied, the large number of lines emitted in the region of $\lambda 4800\text{--}5000 \text{ \AA}$ can make it very difficult to obtain a good profile of H_β . This is especially so at high electron densities when H_β is very broad ($\Delta\lambda_{1/2} \sim 50 \text{ \AA}$ at $N_e = 10^{17} \text{ cm}^{-3}$). Under such conditions the neutral helium line $\lambda 3889 \text{ \AA}$