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TWO PARTICLE EFFECTIVE POTENTIAL OF A DENSE HYDROGENOUS PLASMA

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1 - INTRODUCTION

In many problems dealing with thermodynamic functions and transport properties of a dense fluid or a dense plasma, it is essential to have a precise knowledge of the form of the two-particle effective potential (or binary Slater sum) and the corresponding pair correlation function. Here we consider the simplest case of a gaseous hydrogenous plasma at temperatures high enough for the hydrogen molecules to be dissociated, say about 10^7K. In this system, the classical calculation of the pair radial distribution function g2(r,T)(r.d.f.) diverges when the distance between particles r tends to zero, due to a singularity at r=0. In order to remove this singularity it is necessary to take into account the quantum effects. But, the inclusion of these effects increases considerably the difficulty of calculations. To keep these calculations analytic one has to make some simplifying approximations. Following these lines and for \( k_B T > 1 \) Ryd, Deutsch [1] obtained a Kramers-like pseudo-potential in the framework of the Two-Component Plasma model. In earlier works, with the inclusion of Diffraction [2] and Symmetry effects [3], some formally analogous expressions were derived, in high-temperature and dense classical electron gas within the framework of the One-Component Plasma model. References to previous works on this problem are, by Barker [4], and Davies and Storer [5].

2 - NUMERICAL COMPUTATION

At the present time, an exact calculation of the quantum-mechanical r.d.f. at any separation r is only feasible by means of heavy electronic computations. In this work, which is an extention of Barker's study [4], we are computing numerically \( g_{ep}(r,T), g_{ee}(r,T) \), and their corresponding effective potential at all distances and at different temperatures, with a high accuracy (errors less than one over 10^6). \( g_{ep} \) and \( g_{ee} \) are respectively electron-proton, and electron-electron r.d.f. As two examples of these calculations: figure 1 shows variations of \( g_{ep} \) versus \( rT \) at different temperatures \( T \); while figure 2 illustrate the contribution of \( g_{b} \) and \( g_{g} \) to \( g_{ep} \) at \( T=10^5K \). \( g_{b} \) and \( g_{g} \) are respectively contributions to \( g_{ep} \) from bound states and scattered states of e-p system. In this figure \( g_{c} \) is the r.d.f. corresponding to a Coulomb potential:

\[
g_{c} = \exp \left( -\frac{6e^2}{r} \right) \quad \text{with} \quad \beta = (k_B T)^{-1}
\]

Based on these and other results we obtained the following simple empirical expression, which reproduces quite satisfactorily the exact numerical results:

\[
\ln g_{ep}^{1}(x,y) = \left[ (\gamma/2)^{1/2}/\kappa \right] \{ \exp \left[-(ax + by + Cy^2) \right] - 1 \}
\]

where \( x = r/a \); \( \kappa \) is the thermal De Broglie wavelength \( \kappa = \hbar/(\mu^{1/2}) \); \( \mu \) is the reduced mass;

\[
a = (2\pi)^{1/2} + (\gamma/2)^{1/2} [ (n^2/3) - n ]
\]

\[
+ (2\pi)^{1/2} [ \xi(3)(n/4)^{1/2} + (\gamma/2)^{1/2} (5/36)^{1/2} ]
\]

\[
b = \frac{2}{2} - 2 \quad c = a(b - 2) \quad \text{and} \quad \gamma = 2(e^2/\hbar)^2 \mu \beta
\]

3 - SMALL r REGION

The exact quantum-mechanical expression for r.d.f. can be arranged, after a lengthy calculation, in increasing power of \( r \). The final result for \( g_{ep} \) is:

\[
g_{ep}(x,y) = (\pi n)^{1/2} [ 1 - (2\gamma)^{1/2} x + \gamma x^2 ]
\]

\[
- \frac{2}{9} \left( \frac{\pi}{2} \right)^{3/2} x^3 (5+4D) + \frac{2}{72} x^4 (7 + 20 D) \gamma
\]

\[
- \frac{1}{225} \left( \frac{\pi}{2} \right)^{5/2} x^5 (2(21+140 D) + 64 D^2) \gamma
\]

\[
+ \frac{1}{1350} \pi \left( \frac{\pi}{4} \right)^3 (5 + 35D + 56D^2) \gamma - 0(\gamma^{3/2} x^3)
\]

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where:

$$D_y^n f(\gamma) = \frac{d^n f(\gamma)}{d\gamma^n}$$

when \( r \) is small \((x << l)\), the first few terms of this expression gives a satisfactory approximation of exact \( g_{ep} \).

Finally, we pay attention to the very-high temperature regime, where relativistic effects become non-negligible for plasma with large Z species.

REFERENCES


Figure 1 - Electron-proton radial distribution function \( g_{ep} \) at different temperatures.

Figure 2 - Electron-proton radial distribution function versus \( rT \).

\( g_b \) and \( g_s \) are respective contributions to \( g_{ep} \) from bound states and scattered states.

\( g_c \) is the r.d.f. corresponding to a Coulomb potential.