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2.B Thermodynamics of a Polarizable One-Component Plasma

Introduction

The thermodynamic properties of dense plasmas, of electron density 10^{22} to 10^{26} cm^{-3}, in the temperature range 1 eV to 1 KeV, are not well known. At these high densities, the ion-ion interactions are very strong and generally their contribution to the plasma free energy cannot be regarded as minor.

Further, the ion interactions cannot be easily treated in terms of conventional two-body collision integrals because a typical ion is actually in "strong" collision with several neighboring ions simultaneously. A strong collision is one in which an appreciable part of an ion's kinetic energy is converted into potential energy during the collision. A measure of the importance of strong collisions is provided by the parameter $\Gamma = Ze^2/akT$ (where a is the ion sphere radius, given by $4\pi n_i a^3/3 = 1$). When $\Gamma > 1$, in effect, an ion is always in the strong collision regime; for our purposes the region of interest is $10 > \Gamma > 0.1$.

In addition, the electron-ion interactions contribute appreciable binding energy. Electrons tend to bunch around ions, providing shielding for the ions. This shielding is not very important at extremely high densities because the electrons are then quite degenerate and the Fermi energy (measured by the parameter $b = \mu/kT$, where μ is the chemical potential) greatly exceeds the interaction energy (measured by Γ), resulting in electrons that are fairly uniformly distributed throughout the plasma. At lower densities (measured by the parameter $b/\Gamma \sim 1$), and

at higher temperatures or smaller values of Γ, electrons are only partially degenerate and bunching around ions takes place, thereby polarizing the plasma.

High-density plasmas have been represented by a model consisting of pointlike ions embedded in a uniform electron background, called the one-component plasma (OCP). The OCP has been studied intensively by a number of investigators[1] because it simulates low temperature, high density, and fully ionized plasmas – yet its thermodynamic properties are simplified, being a function of just the one parameter Γ. Monte Carlo techniques are used to evaluate the complicated ion-ion interactions. While the OCP can model very high-density plasmas, its range of applicability can only be determined by comparison with a more physical plasma model. In our present work we do so and find that deviations in the estimates of the internal energy and pressure start appearing when the ion density falls appreciably below 9×10^{28} cm^{-3}. The purpose of these calculations is to supplement these classical OCP investigations by determining the thermodynamic properties of dense plasmas that are only partially degenerate. This work extends similar calculations by DeWitt and Hubbard[2] and Totsuji and Takami.[3] An additional purpose is to determine radial distribution functions for partially degenerate plasmas; these can be used for testing theoretical methods of calculating plasma properties.

The Calculation

The thermodynamic properties result from evaluation of derivatives of the free energy, or of the partition function, with respect to temperature and density. To evaluate $U = -(\partial \ln \hat{Z}/\partial\beta)_V$, $\beta P = (\partial \ln \hat{Z}/\partial V)_T$, etc., we start with N pointlike ions and the expression for the partition function:

$$\hat{Z} = e^{-\beta F_{ions}} \cdot \int \frac{d^{3N}R}{V^N} e^{-\beta U_{ii}} \mathrm{Tr}\left[e^{-\beta(K_e + U_{ee} + U_{ie})} \right]. \quad (1)$$

The plasmas are assumed completely ionized; this assumption limits the applicability of the present phase of this work. Following a procedure discussed by Ashcroft and Stroud,[5] the trace in the integral may be evaluated when the electron density fluctuations are linear in the electric potential, as, for instance, $\delta\tilde{\rho}(k) = q^2\eta(k)\tilde{\varphi}(k)$ (where the tilde signifies the Fourier transform), and the Helmholtz free energy can then be calculated.

The dielectric function was calculated using the linear form of a density matrix, a procedure developed by March and Murray;[6] this gives

$$q^2\eta(k) = \frac{4}{\pi a_{Bohr} k} \int_0^\infty \frac{k'}{1 + \exp[\beta[E(k') - \mu]]} \ln\left| \frac{k + 2k'}{k - 2k'} \right| dk'. \quad (2)$$

Here, μ is the chemical potential and $k^2[\epsilon(k) - 1] = q^2\eta(k)$.

This form is in agreement with the random phase approximation (RPA) dielectric function used by Totsuji and Takami.[3] The potential closely approximates exp(-qr)/r, where q is the Thomas-Fermi wave number. There are additional oscillatory terms, of order r^{-3}, which amount to a few percent for values of r that are of interest (see Fig. 28.7). These minor Friedel oscillation terms can provide long-term coupling of the plasma at distances greater than a few ion-sphere radii.

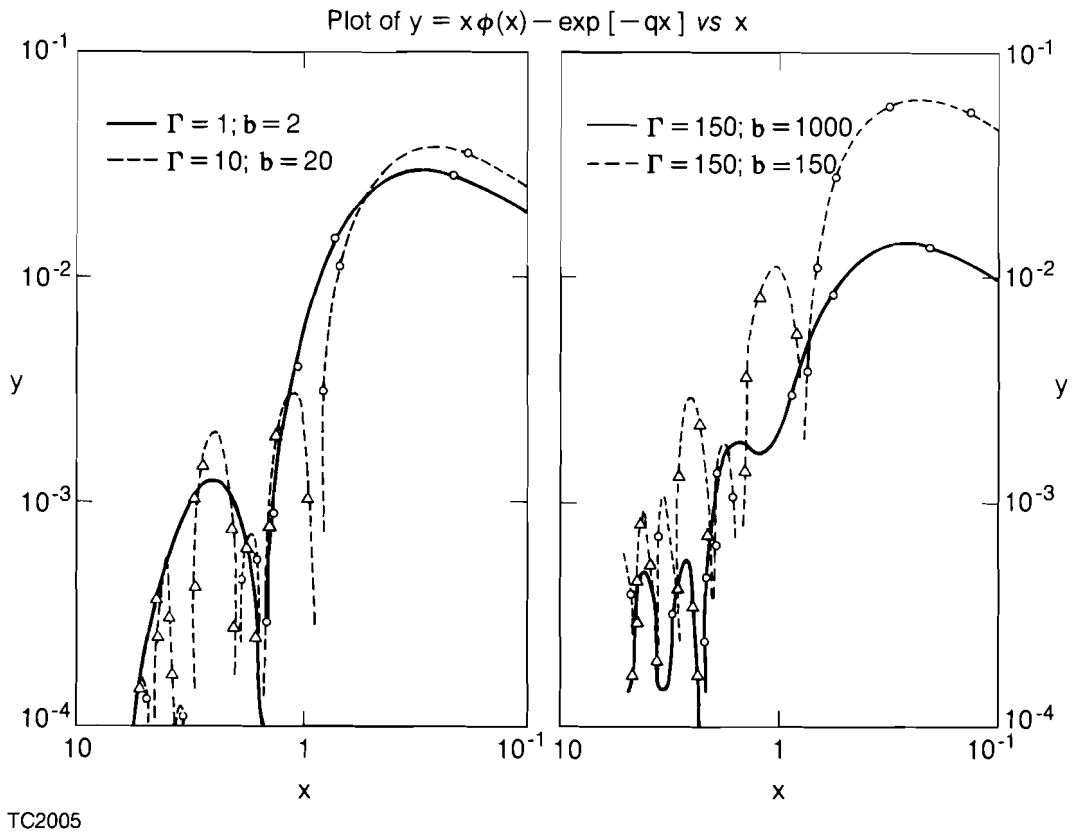

Fig. 28.7
Departures of the calculated potential from a Yukawa potential. Here, x = r/a, where a is the ion-sphere radius. (The usual plasma density parameter, $r_s = a/a_{Bohr}$, is given by $r_s \sim 2\,\Gamma/b$.)

One gets $\hat{Z}$ in a form useful for performing a Monte Carlo calculation:

$$\hat{Z} = e^{-\beta[F_{\text{(ideal ions)}} + F_{\text{(free electrons)}} + F_{\text{pol}}]} \cdot \int \frac{d^{3N}R}{V^N} e^{-\beta U_{\text{eff}}}, \qquad (3)$$

where

$$\beta U_{\text{eff}} = \frac{1}{2}\beta \left\{ \sum_{I \neq J} \sum Z_I Z_J \phi\left(|R_I - R_J|\right) + \sum_I Z_I^2 \lim_{\xi \to 0} \left[\phi(\xi) - \frac{1}{\xi}\right] \right\}, \qquad (4)$$

and

$$\tilde{\phi}\,(k) = \frac{4\pi}{k^2 + q^2\,\eta\,(k)} \quad . \tag{5}$$

For the plasmas presently being considered, F_{pol} is a small second-order term that can be ignored. The calculations use an Ewald sum technique for calculating U_{eff} and evaluating the pair distribution function. In effect, the plasma is represented as a cubic lattice, with N (= 128) ions per cell. For details, see Ref. 7.

In addition to the ordinary internal energy and pressure terms associated with noninteracting electron and ion gases, there are excess energy and pressure terms attributable to the interactions; these are

$$\frac{\beta U_{excess}}{N} \cong < \frac{\beta U_{eff}}{N} > \quad ; \tag{6}$$

$$\frac{\beta V P_{excess}}{N} \cong \frac{1}{3}\left(1 + \frac{1}{2} <qr>\right) < \frac{\beta U_{eff}}{N} > + \frac{1}{12} Z^2 \Gamma q^* a \quad ; \tag{7}$$

where $<U_{eff}/N>$ and $<qr>$ are quantities resulting from the Monte Carlo calculation, and q^* is calculated from the limiting value of the effective two-body potential when $r \rightarrow 0$. Here, a is the ion sphere radius.

Results

Figure 28.8 shows the excess-energy term. It has been divided into two parts: (1) the energy per ion of a reference rigid body-centered cubic lattice (BCC); and (2) the difference in energy per ion between the plasma and the BCC lattice.

At large Γ the BCC lattice energy dominates. The BCC excess energy decreases from the OCP value as the density decreases. This reflects the binding energy of the electrons as they cluster around individual ions. For the plasmas studied, the difference in excess energy, plasma to lattice, also decreases with density, amounting to 0.5 kT per ion at ion densities of 2×10^{23} cm^{-3} (for Z = 1). The difference in energies is not a strong function of Γ at low densities. The very low-density, high-Γ models may be quite unphysical because deionization is not taken into account; for these models the plasma excess energy is less than that of the BCC lattice.

The excess-pressure terms must be tabulated. For the OCP, the terms involving q and q^* are absent in the expression for the excess pressure. The extra terms can cause the excess pressure to be more negative by up to 20% than in the OCP case. The calculations show that the following crude approximations may be used:

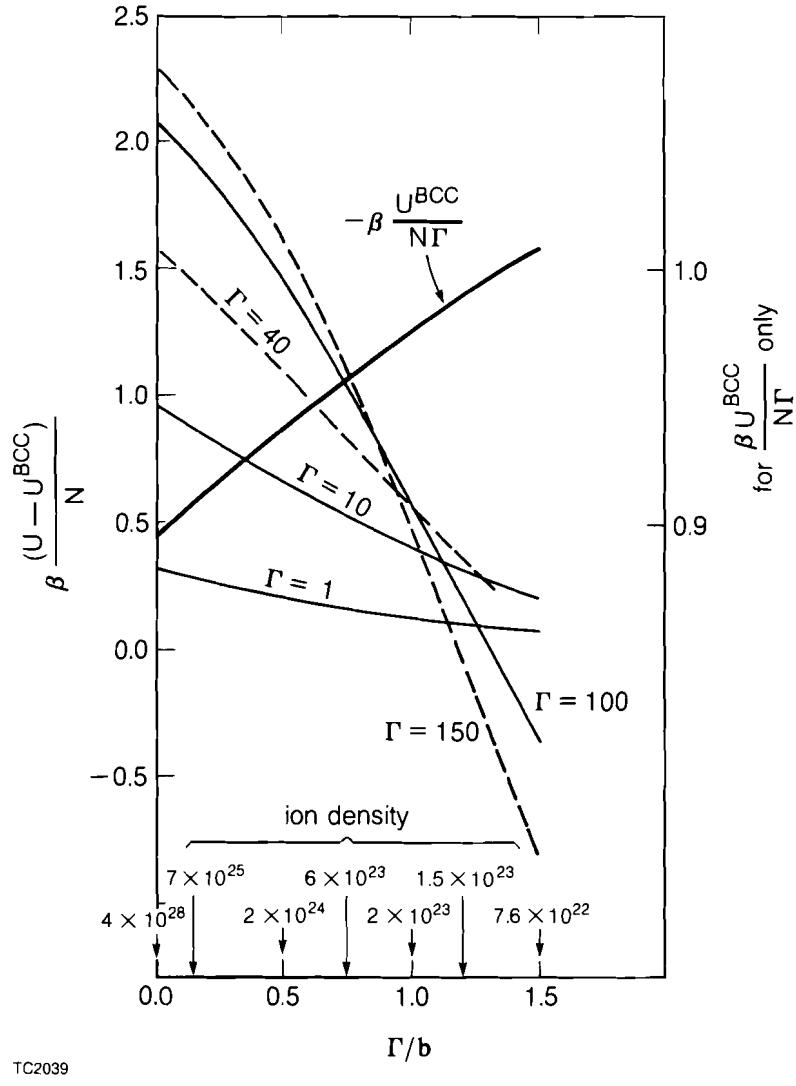

Fig. 28.8
Excess energies vs $\Gamma/b(= \Gamma kT/\mu \cong 0.5r_s)$. The heavy solid line refers to a reference BCC lattice and the scale on the right. The other curves, for constant Γ , refer to the scale on the left.

$$< \frac{\beta U_{eff}}{N} > \sim -(0.9 + 0.033 r_s)\,\Gamma Z^2 \quad \text{where } r_s = a/a_{Bohr} , \tag{8}$$

and

$$<qr> \sim \min(\frac{2}{3} qa, 2) \text{ and } q^* \sim q. \tag{9}$$

The pair-correlation functions show some unusual features (see Fig. 28.9). The minor oscillations beyond the first maximum first decrease in amplitude as one goes to lower densities and then increase in strength

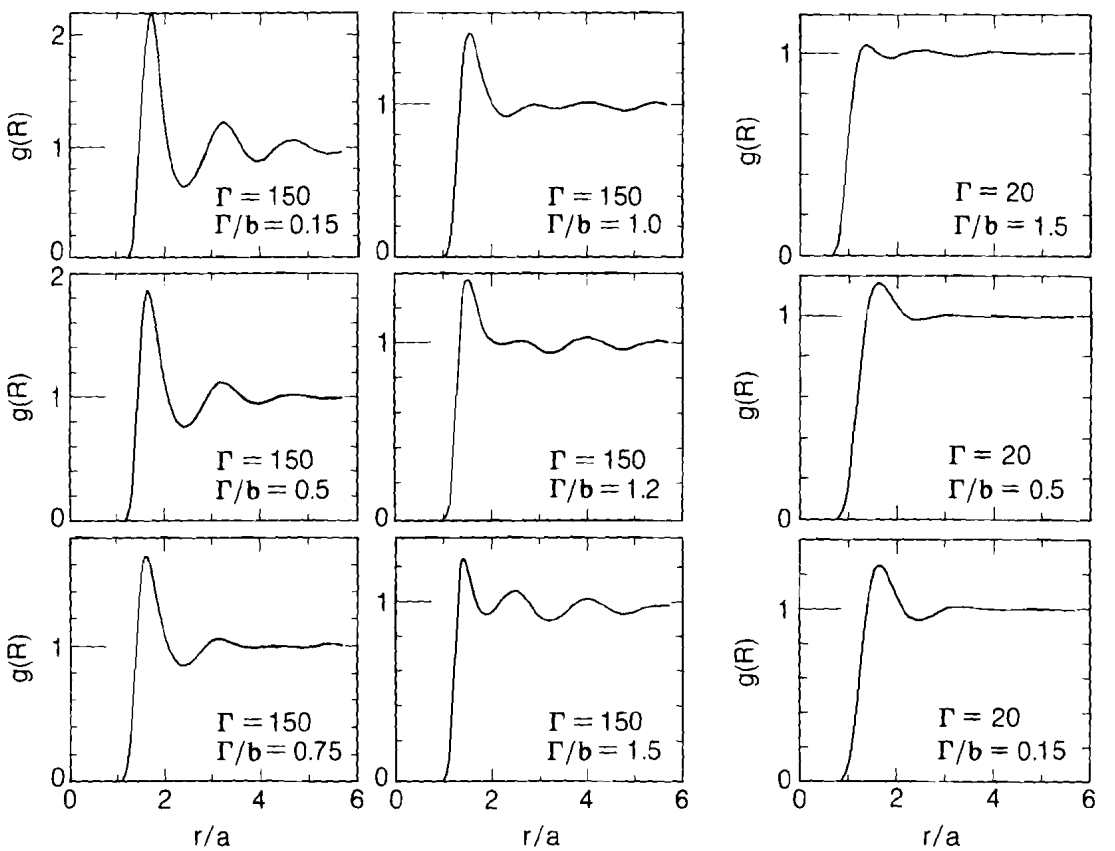

Fig. 28.9
Pair-correlation functions vs r/a, where a is the ion-sphere radius. The various curves are labeled by a density parameter (see Fig. 28.8).

(with a phase shift) as one goes to the lowest densities studied. This behavior is for all the models, down to the lowest value of Γ for which the oscillations can be studied. A modern theoretical interpretation, based on using the modified hyper-netted chain equation, will be tried in the future.

This work is basically complete from Γ = 200 to 1, and r_s = 0 to 3 (here $r_s = a/b_{Bohr}$) and for Z = 1. The extension to the extremely interesting high-temperature regime, Γ = 0.01 to Γ = 1, requires supercomputer time because extensive tables must be stored in order to calculate the necessary temperature and density derivatives.

ACKNOWLEDGMENT

The work was supported by the National Science Foundation under grant No. PHY-8406878.