Low density free energy of two-dimensional real matter

1980 J. Phys. A: Math. Gen. 13 L197

(http://iopscience.iop.org/0305-4470/13/6/007)

J. Phys. A: Math. Gen., 13 (1980) L197–L199. Printed in Great Britain

LETTER TO THE EDITOR

Low density free energy of two-dimensional real matter

C Deutsch

Laboratoire de Physique des Plasmas†, Université Paris-Sud, 91405 Orsay, France

Received 24 March 1980

Abstract. The canonical thermodynamics of the system of electrons interacting with nuclei in a plane, through the r^{-1} potential, is investigated within the mean field (Debye) theory. The free energy per particle in the high dilution ($\rho \to 0$) limit behaves as $k_B T \Lambda (A \ln \Lambda + B)$.

We consider the thermodynamics of the two-dimensional and two-component electron–ion system interacting in a plane via the three-dimensional Coulomb law r^{-1}.

This two-dimensional model of real matter is of considerable intrinsic interest, in view of its relevance to semiconductor physics (metal–oxide sandwiches) (Stern and Howard 1967) and controlled fusion physics (behaviour of the pellet surface in the energy transfer process).

We intend to pay particular attention to the thermodynamics of this system in the high-dilution and high-temperature limits, where $k_B T$ is comparable to or not much smaller than the hydrogen binding energy.

Our purpose is to compare the present results with those already known for the corresponding one-component plasma (OCP) model (Chalupa 1975, Totsuji 1976).

In view of the important technical difficulties associated with the adaptation of the OCP nodal expansion in $\Lambda = 4\pi\rho\, e^4 (k_B T)^{-2}$ of the canonical thermodynamics to the two-component plasma (TCP), we shall start from another perturbative formulation where the unperturbed state is the perfect gas of N non-interacting neutral pairs rather than the perfect gas of $2N$ charges of either sign (Baer 1970). This alternative approach stresses the distinction (Lebowitz *et al* 1965) between the residual weak long-range interaction for particles pertaining to distinct atoms, and the strong short-ranged quantum interaction within a pair of like charges.

In the present scheme, the Debye approximation appears as a long-range resummation of the r^{-1} interaction between charges located on distinct atoms. In diagrammatic language, the only change from the OCP resummation (Deutsch 1978) is the replacement of a particle vertex by a neutral pair vertex at each field (nodal) point.

In the small ρ range, one can therefore compute (Baer 1970) the pair correlations $f_{\alpha\beta}$ from the zero-order distribution $f^0_{\alpha\beta}$ for a pair of charges at two distinct positions and two imaginary times: $0 \leqslant \tau \leqslant \beta = (k_B T)^{-1}$, with the translational molecular motion factorised out ($\alpha, \beta = e, i$). f^0_{ie} and f^0_{ee} are τ-independent. We also neglect the τ-dependence of f^0_{ee}. So, we get $f^0_{ee} = f^0_{ii}$, which amounts to neglecting all effects of instantaneous charge fluctuations inside the 'atoms' on the interaction among them. The divergence at $T \to \infty$ of $f^0_{ii} = f^0_{ee} \sim \mathrm{Tr}(e^{-\beta H})_c$ can be avoided by noticing that the $f^0_{\alpha\beta}$

† Laboratory associated with the CNRS.

0305-4470/80/060197+03$01.50

are zero-order approximations to the intra-atomic correlations. The self-correlations at $\tau = 0$ are

$$f_{ii} = f_{ee} = \rho\delta(\boldsymbol{r}). \tag{1}$$

It then remains to compute $f_{ei}(r)$. At $\tau = 0$, the $f^0_{\alpha\beta}$ represent the zero-order terms of the pair correlation functions $F_{\alpha\beta}(r)$.

Following the Baer convention, we represent $f_{\alpha\beta}$ graphically by a big circle with two root points labelled by α and β. Dropping one or two of the labels corresponds to a diagrammatic representation of

$$f_\alpha = \sum_\beta e_\beta f_{\alpha\beta}, \qquad f = \sum_{\alpha,\beta} e_\alpha e_\beta f_{\alpha\beta}, \tag{2}$$

respectively, where e_α is the electric charge on the αth particle. The resummation of the Coulomb tail is now monitored by convolution chains of alternate f functions (big circles) and $-1/r$ functions (lines), with f_α and f_β at the two ends of the chain. Every 'black' (intermediate) point represents an integration over space coordinates, and every pair of black end-points of a line represents an additional integration over a τ variable. Every 'white' (root) point represents a fixed space coordinate and value. The formal summation of the chain diagrams can be obtained from $\tilde{f}(k)$, the Fourier transform of $f(r)$.

For this purpose, it is convenient to introduce the sum of the four binary correlations

$$F(r) = \sum_{\alpha,\beta} e_\alpha e_\beta F_{\alpha\beta}(r).$$

The Debye procedure thus yields

$$\tilde{F}(k) = \tilde{f}(k)\left(1 + \frac{2\pi\beta\tilde{f}}{k}(k)\right)^{-1}, \tag{3}$$

where we make use of $2\pi/k$, the Fourier transform of r^{-1}. β^n follows from the τ-integration in the nth chain. From equation (1) one obtains

$$F_{ii} = F_{ee}, \qquad F = 2e^2(F_{ii} - F_{ie}). \tag{4}$$

The large-r behaviour of $F(r)$ is obtained from

$$f(r) = 2\rho e^2(\delta(r) - \rho q_\mu^{-1} S(r)_c), \tag{5}$$

where $q_\mu = \mu/2\pi\beta\hbar^2$ with μ the electron–ion reduced mass, while $S(r) \equiv \langle \boldsymbol{r}|e^{-\beta H}|\boldsymbol{r}\rangle$ is the atom Slater sum. Splitting up the Hamiltonian in $S(r)$ into the kinetic and the potential parts, $H = H_0 - Ze^2/r$, we take the two parts as commutable for large r, so that

$$\lim_{r\to\infty} S(r) = \langle \boldsymbol{r}|\exp(-\beta H_0)|\boldsymbol{r}\rangle \exp(\beta Z e^2/r) = q_\mu \exp(\beta Z e^2 r^{-1}). \tag{6}$$

Asymptotically, $S(r)_c = q_\mu(\beta Z e^2/r)$. This expression is valid for $r \gg \max(\beta e^2, \hbar/(2\pi\mu k_B T)^{1/2})$. Using equation (12) in equation (11), we obtain for this r range

$$f(r) = \delta(r)/\rho - \beta Z e^2/r. \tag{7}$$

$\tilde{F}(k)$ is thus obtained as ($K = 4\pi\beta\rho e^2$)

$$\tilde{F}(k) = \frac{1}{\rho} + 8\pi\beta e^2 \frac{(K - 3k)}{(k - K_0)(k + K_S)}, \tag{8}$$

where $2K_0 = K(\sqrt{3}-1)$ and $2K_S = K(\sqrt{3}+1)$. Equation (8) is then valid for $k \ll (\beta e^2)^{-1}$ and $K \ll (\beta e^2)^{-1}$, i.e. when $\Lambda \ll 1$ or $\rho \to 0$ and $T \to \infty$. When these two requirements are fulfilled, equation (8) may be safely taken as a reliable approximation in the whole k range.

Taking the principal part of the Fourier integral yields

$$F(r) = \delta(r)/2\pi\rho + \Lambda[-3/r + (H_0(K_0r) + N_0(K_0r))K_0\alpha(K_0) + (H_0(K_Sr) - N_0(K_Sr))K_S\alpha(K_S)] \tag{9}$$

in terms of the Struve function $H_0(x)$ and the Neumann function $N_0(x)$ with K_0 and K_S now in number of K, and r in K^{-1}, while

$$\alpha(K_0) = \pi(5-3\sqrt{3})/2\sqrt{3}, \qquad \alpha(K_S) = \pi(5+3\sqrt{3})/2\sqrt{3},$$

and the asymptotic behaviour

$$\lim_{r\to\infty} F(r) \simeq \Lambda\left[-\frac{\sqrt{3}(\sqrt{3}-1)}{r} + K_0\alpha(K_0)\frac{2\sqrt{2}}{(\pi K_0 r)^{1/2}}\sin\left(K_0r - \frac{\pi}{4}\right) - \frac{2}{\pi}\frac{\alpha(K_0)K_0}{(K_0r)^3} - \frac{K_S\alpha(K_S)}{(K_Sr)^3}\frac{2}{\pi}\right]. \tag{10}$$

This last result is typical of the present 'molecular' approach (Deutsch 1975) with an unscreened long-ranged oscillatory tail (Baer 1970). However, as in three dimensions, the canonical internal energy

$$E/Nk_BT = \tfrac{1}{4}\Lambda[\tfrac{1}{2}(K_0\alpha(K_0) + K_S\alpha(K_S)) + (2/\sqrt{3})(1+\sqrt{3})\ln\Lambda + (2/\sqrt{3}-1)(\tfrac{1}{8}\pi - \ln 2)] \tag{11}$$

does not depend on this dipole-like oscillatory contribution to $F(r)$. Equation (11) is qualitatively analogous to its OCP homologue (Totsuji 1976).

References

Baer S 1970 *Phys. Rev.* A **2** 2454
Chalupa F 1975 *Phys. Rev.* B **12** 4
Deutsch C 1975 *Strongly Coupled Plasmas* ed G Kalman (New York: Plenum) p 315
—— 1978 *Ann. Phys., NY* **115** 404
Lebowitz J L, Stell G and Baer S 1965 *J. Math. Phys.*
Stern F and Howard W E 1967 *Phys. Rev.* **163** 816
Totsuji H 1976 *J. Phys. Soc. Japan* **40** 857