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The Two-Dimensional One-Component Plasma at $\Gamma = 2$: The Semiperiodic Strip

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The one-component two-dimensional plasma is studied in a strip of finite width, replicated periodically parallel to the long axis of the strip. Exact results for the one- and two-particle distribution functions are found at coupling $\Gamma = q^2/kT = 2$. The system is inhomogeneous: the one- and two-particle distribution functions show long-range order.

KEY WORDS: Long-range order; semiperiodic boundary conditions; two-dimensional–one-component plasma.

Recently, several papers[1–7] have discussed exact properties of the two-dimensional one-component plasma at a particular temperature. The system is composed of a region Λ containing N particles of charge q and a uniform background charge density $-\rho q$. The system has zero net charge so that $N = \rho|\Lambda|$. The energy of a configuration $\{\mathbf{r}_1, \ldots, \mathbf{r}_N\}$ of the charges is

$$E(\{\mathbf{r}_1, \ldots, \mathbf{r}_N\}) = \tfrac{1}{2}q^2\left\{ \sum_{j=1}^{N} \lim_{\mathbf{r}\to\mathbf{r}_j}\left[\Phi(\mathbf{r}) + \tfrac{1}{2}\log(\mathbf{r}-\mathbf{r}_j)^2\right] - \rho\int_\Lambda d^2\mathbf{r}\,\Phi(\mathbf{r})\right\} \tag{1}$$

Here the function Φ is the solution of

$$\nabla^2\Phi(\mathbf{r}) = -2\pi\left\{\sum_{j=1}^{N}\delta(\mathbf{r}-\mathbf{r}_j) - \rho\right\} \tag{2}$$

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together with some boundary condition on $\partial\Lambda$ or perhaps at infinity. The particular temperature at which exact results are available is given by $\Gamma = q^2/kT = 2$: it is possible to calculate the one- and two-particle distribution functions exactly, as well as the partition function. The results are interesting for a number of reasons, not the least being that they are a rare example of an exactly soluble continuous system in more than one dimension. A more concrete reason for interest in the results is that they provide an exact standard against which to test approximate theories and simulation results for ionic systems. This idea applies particularly to studies of surface properties. In a very general context, the exact results have helped form the new qualitative insights given by sum rules in ionic systems[2, 3, 8–10]. They have been most valuable in clarifying the nature of the large-distance asymptotic decay of the truncated two-particle distribution function along boundaries in semi-infinite systems. In finite-width strips, exact results show even more complex behavior in this long-range decay.[7]

It may be expected then, that exact calculations on a system with periodic boundary conditions will be of considerable use in establishing a correct interpretation of the results of computer simulations using periodic boundary conditions. Such an exactly soluble system has been found[11] and we discuss some of its properties here.

Consider the N particles discussed above in a rectangle Λ with $\mathbf{r} = (x, y) \in \Lambda$ if $-L/2 \leqslant x \leqslant L/2$ and $-W/2 \leqslant y < W/2$. The potential $\Phi((x, y))$ of Eq. (2) may be calculated by writing Φ as a Fourier series in y. Thus Φ is periodic in y with period chosen to be W. The series coefficients are functions of x and written as inverse Fourier transforms. The charge density on the right-hand side of (2) is expanded in the same way and the solution found by equating coefficients. This solution allows the potential energy E of Eq. (1) to be written in the form[11]

$$E(\{\mathbf{r}_1, \ldots, \mathbf{r}_N\}) = q^2 \sum_{j=1}^{N-1} \sum_{k=j+1}^{N} \phi(\mathbf{r}_j, \mathbf{r}_k) + \pi\rho q^2 \sum_{j=1}^{N} x_j^2 + B_N \tag{3}$$

Here, B_N is a constant, irrelevant to the distribution functions, and

$$\begin{aligned}\phi(\mathbf{r}_1, \mathbf{r}_2) = &-\frac{\pi}{W}|x_1 - x_2| \\ &-\frac{1}{2}\log\left\{1 - 2\exp\left[-\frac{2\pi}{W}|x_1 - x_2|\right]\cos\frac{2\pi}{W}(y_1 - y_2) \right. \\ &\left. + \exp\left[-\frac{4\pi}{W}|x_1 - x_2|\right]\right\}\end{aligned} \tag{4}$$

The term proportional to $|x_1 - x_2|$ comes from the $n = 0$ term in the

Fourier series solution of (2), while the other terms sum to give the logarithmic part of (4).

This energy may be inserted into the standard formula for the canonical partition function $Z_N(\Gamma)$ at $\Gamma = 2$. We then order the x variables. This may be done in $N!$ equivalent ways. Using the ordering $-(L/2) \leqslant x_1 \leqslant x_2 \leqslant \cdots \leqslant x_N \leqslant L/2$ gives

$$Z_N(2) = e^{-\beta B_N} \int_{-L/2}^{L/2} dx_N \int_{-L/2}^{x_N} dx_{N-1} \cdots \int_{-L/2}^{x_2} dx_1 \exp\left(-2\pi\rho \sum_{j=1}^{N} x_j^2 \right)$$
$$\times \int_{-W/2}^{W/2} dy_1 \cdots \int_{-W/2}^{W/2} dy_N$$
$$\times \prod_{j=1}^{N-1} \prod_{k=j+1}^{N} \left(\exp\left[\frac{2\pi}{W}(x_j + x_k) \right] \right.$$
$$\times \left| \left\{ \exp\left[-\frac{2\pi}{W}(x_k - iy_k) \right] \right. \right.$$
$$\left. \left. \left. - \exp\left[-\frac{2\pi}{W}(x_j - iy_j) \right] \right\} \right|^2 \right) \tag{5}$$

Notice that the y-dependent part of the integrand is contained in the square modulus of a van der Monde determinant. We use the permutation notation $P\{1,2,\ldots,N\} = \{P(1), P(2), \ldots, P(N)\}$ for a permutation with signature $\epsilon(P)$ to write down the expansion of the determinant and its conjugate. This procedure gives

$$\int_{-W/2}^{W/2} dy_1 \cdots \int_{-W/2}^{W/2} dy_N \prod_{j=1}^{N-1} \prod_{k=j+1}^{N}$$
$$\times \left| \left\{ \exp\left[-\frac{2\pi}{W}(x_k - iy_k) \right] - \exp\left[-\frac{2\pi}{W}(x_j - iy_j) \right] \right\} \right|^2$$
$$= \sum_{P=1}^{N!} \sum_{Q=1}^{N!} \epsilon(P)\epsilon(Q) \prod_{j=1}^{N}$$
$$\times \left(\exp\left\{ -\frac{2\pi x_j}{W} \left[P(j) + Q(j) - 2 \right] \right\} \right.$$
$$\left. \times \int_{-W/2}^{W/2} dy_j \exp\left\{ -\frac{2\pi i}{W} y_j \left[P(j) - Q(j) \right] \right\} \right)$$

Only permutations for which $P(j) = Q(j)$, $1 \leqslant j \leqslant N$ contribute.

We obtain

$$Z_N(2) = W^N \exp(-\beta B_N) \sum_{P=1}^{N!} \int_{-L/2}^{L/2} dx_N \int_{-L/2}^{x_N} dx_{N-1} \cdots \int_{-L/2}^{x_2} dx_1$$
$$\times \prod_{j=1}^{N} \exp\left(-2\pi\rho\left\{ x_j^2 - 2x_j \frac{L}{2}\left[1 - \frac{2P(j)-1}{N}\right]\right\}\right)$$

For permutation P, make the substitution $x_j = z_{P(j)}$, $1 \leqslant j \leqslant N$. We then have a sum over ordered integrals over the z_j. The integrand is the same for each permutation and each possible ordering of the z_j occurs exactly once. Hence, the sum over ordered integrals may be written as an unrestricted multiple integral over $[-L/2, L/2]^N$. Renaming $z_j = x_j$ for $1 \leqslant j \leqslant N$ and using the appropriately defined C_N, we obtain

$$Z_N(2) = W^N \exp(-\beta C_N) \prod_{j=1}^{N} \int_{-L/2}^{L/2} dx_j$$
$$\times \exp\left\{-2\pi\rho\left[x_j - \frac{L}{2}\left(1 - \frac{2j-1}{N}\right)\right]^2\right\} \tag{6}$$

Using the correct form of C_N we may now take the thermodynamic limit of $-[\log Z_N(2)]/N$ to obtain the free energy per particle. We let $L \to \infty$ with $N/LW = \rho$ and obtain for the free energy

$$\beta f(2) = \beta f_0(2) + M \tag{7}$$

where $M = \pi/6\rho W^2$ is a Madelung constant for the potential in the semiperiodic boundary conditions used here at $\Gamma = 2$. The function $f_0(2)$ is Jancovici's[1] thermodynamic limit free energy per particle,

$$f_0(2) = \log \rho \lambda_D^2 - \tfrac{1}{2}\log 2 - \tfrac{1}{2}\log \rho W^2/4 \tag{8}$$

for the system confined to a disc. Here λ_D is the de Broglie wavelength and we have set Jancovici's scaling length $L_0 = W/2\pi$. Equation (6) describes the canonical partition function for an assembly of N independent harmonic oscillators with mean positions evenly spaced on $[-L/2, L/2]$.

To calculate the one-particle distribution function we simply leave out the integrations over x and y. Define $x_0 = -L/2$, $x_{N+1} = L/2$, and the T_p ordering as an ordering of the x variables with $x_0 \leqslant x_2 \leqslant x_3 \leqslant \cdots \leqslant x_p \leqslant x_1 < x_{p+1} \leqslant \cdots \leqslant x_N \leqslant x_{N+1}$. There are $(N-1)!$ orderings, each giving the same contribution to $\rho_{(1)}(x, y)$. We use the van der Monde determinant representation of the integrand and carry out the integrations over $y_2, \ldots, y_N$ giving $P(j) = Q(j)$, $2 \leqslant j \leqslant N$, and so $P(1) = Q(1)$ by default. Collect all the integrals with $P(1) = q$ and change variables with

$x_j = z_{P(j)}$, $2 \leqslant j \leqslant N$; $P(j) \neq q$ and $x_1 = z_q$. This generates ordered integrals with respect to $(N-1)$ of the z_j, all possible orderings occurring exactly once. An unrestricted integral over

$$\{z_1, \ldots, z_{q-1}, z_{q+1}, \ldots, z_N\} \in [-L/2, L/2]^{N-1}$$

results. The final form for the one-particle distribution function is then

$$\rho_{(1)}(\mathbf{r}; N) = \frac{1}{W} \sum_{q=1}^{N} \exp\left\{ -2\pi\rho\left[x_1 - \frac{L}{2}\left(1 - \frac{2q-1}{N}\right)\right]^2\right\} \Big/ I(q, L, N) \tag{9}$$

where

$$I(q, L, N) = \int_{-L/2}^{L/2} dx \exp\left\{ -2\pi\rho\left[x - \frac{L}{2}\left(1 - \frac{2q-1}{N}\right)\right]^2\right\} \tag{10}$$

This pair of formulas is remarkable in that it gives a closed-form result for the one-particle distribution function, even for a finite system. The result is simpler than the one-dimensional case.(12) Our method reduces the system to a set of N independent harmonic oscillators by using the second-ordering transformation $x_j \to z_{P(j)}$ described above. In the one-dimensional case this second transformation does not appear and that system reduces to a set of N-ordered but otherwise independent harmonic oscillators. A connection with the one-dimensional system may be seen in the $|x_1 - x_2|$ term in the pair potential in Eq. (4).

To obtain the two-particle distribution function, the x_1, y_1 and x_2, y_2 integrations must be omitted. The integrations are written as sums over $T_{p_1p_2}$-ordered x integrations. Under $T_{p_1p_2}$ we have

$$x_0 \leqslant x_3 \leqslant \cdots \leqslant x_{p_1} \leqslant x_1 < x_{p_1+1} \leqslant \cdots \leqslant x_{p_2}$$
$$\leqslant x_2 < x_{p_2+1} \leqslant \cdots \leqslant x_n \leqslant x_{N+1}.$$

We may have $p_1 = p_2$ and then must consider both $x_1 < x_2$ and $x_2 < x_1$. When the y integrations are performed on the van der Monde determinant representation of the y-dependent part of the integrand, the condition $P(j) = Q(j)$, $3 \leqslant j \leqslant N$ is obtained.

There are two classes of terms: those with $P(1) = q_1$, $P(2) = q_2$, $Q(1) = q_1$, $Q(2) = q_2$ in which case $\epsilon(P) = \epsilon(Q)$ and those with $P(1) = q_1$, $P(2) = q_2$, $Q(1) = q_2$, $Q(2) = q_1$ when $\epsilon(P) = -\epsilon(Q)$. A sum over q_1 and $q_2 \in [1, N]$ must be constructed with $q_1 \neq q_2$. Examination of the sum shows that the $q_1 = q_2$ terms would be zero, so they are included. The sum may then be factorized to give

$$P_{(2)}(\mathbf{r}_1,\mathbf{r}_2;N) = P_{(1)}(\mathbf{r}_1;N)P_{(1)}(\mathbf{r}_2;N) - W^{-2}\exp\left[-\pi\rho(x_1-x_2)^2\right] \times\left|\sum_{q=1}^{N}\exp\left\{-2\pi\rho\left[\frac{x_1+x_2}{2}-\frac{L}{2}\left(1-\frac{2q-1}{N}\right)\right]^2 + 2\pi iq(y_1-y_2)/w\right\}\Big/ I(q,L,N)\right|^2 \quad (11)$$

We may now consider the limit $N\to\infty$, $L\to\infty$ such that $\rho = N/LW$ is constant, in which we obtain the infinite strip system distribution functions $\rho_{(1)}(\mathbf{r})$ and $\rho_{(2)}(\mathbf{r}_1,\mathbf{r}_2)$. It is convenient to introduce $\lambda = y/w$, $\xi = \rho W^2$ and $\zeta = x\xi/W$. The parameter ξ measures the number of particles in a square of side W. We obtain a thermodynamic limit for the states in two subsequences, $N = 2M+1$ and $N = 2M$. The results may be written

$$\rho_{(1)}(W\zeta/\xi) = \frac{1}{W^2}F(\zeta,\xi) \quad (12a)$$

and

$$\rho_{(2)}\left(\frac{W\zeta_1}{\xi},\frac{W\zeta_2}{\xi},\lambda\right) = \frac{1}{W^4}\left\{F(\zeta_1,\xi)F(\zeta_2,\xi) - \exp\left[-\frac{\pi}{\xi}(\zeta_1-\zeta_2)^2\right]G\left(\frac{1}{2}(\zeta_1+\zeta_2;\lambda;\xi)\right)\right\} \quad (12b)$$

On the thermodynamic limit subsequence $N = 2M+1$ we have

$$F(\zeta,\xi) = (2\xi)^{1/2}\sum_{l=-\infty}^{\infty}\exp\left[-2\pi(l-\zeta)^2/\xi\right] \quad (13o)$$

and

$$G(\zeta;\lambda;\xi) = 2\xi\left|\sum_{l=-\infty}^{\infty}\exp\left[-2\pi(l-\zeta)^2/\xi + 2\pi il\lambda\right]\right|^2 \quad (14o)$$

On the limit subsequence $N = 2M$ we have

$$F(\zeta,\xi) = (2\xi)^{1/2}\sum_{l=-\infty}^{\infty}\exp\left[-2\pi(l+\tfrac{1}{2}-\zeta)^2/\xi\right] \quad (13e)$$

and

$$G(\zeta;\lambda;\xi) = 2\xi\left|\sum_{l=-\infty}^{\infty}\exp\left[-2\pi(l+\tfrac{1}{2}-\zeta)^2/\xi + 2\pi il\lambda\right]\right|^2 \quad (14e)$$

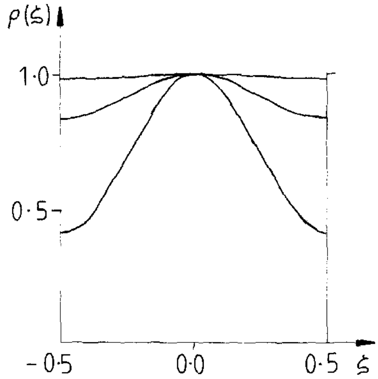

Fig. 1. Plots of $\rho(\zeta) = F(\zeta,\xi)/F(0,\xi)$ for $-1/2 < \zeta < 1/2$. From the bottom upwards the curves are for $\xi = 1.0, 2.0, 2\sqrt{3}$.

Note that the system is inhomogeneous and periodic in the x direction. The inhomogeneity results from the $n = 0$ term in the Fourier series for the potential, which behaves as a potential for a one-dimensional one-component plasma, also known to be periodic. The function $F(\zeta,\xi)$ has unit period in ζ, which means that the period of $\rho_{(1)}(x)$ is $W/\xi = 1/\rho W$. As $W \to \infty$ at ρ fixed, the period decreases to zero, as expected. We plot $F(\zeta,\xi)/F(0,\xi) \equiv \rho(\zeta)$ for $\zeta \in [-\frac{1}{2},\frac{1}{2}]$ in Fig. 1 for three values of ξ. At $\xi = 1$ the density profile shows strongly developed layers. The layers are much less prominent at $\xi = 2$, and at $\xi = 2\sqrt{3}$ the effect is almost absent. Thus as ξ increases at fixed ρ because W increases, we see that the density becomes constant, the correct behavior for the $W \to \infty$ bulk limit. However, for all ξ the one-particle distribution function, in the thermodynamic limit of an infinitely long strip, is a nonconstant periodic function.

Define now the functions

$$H(\zeta;\lambda;\xi) = F(0,\xi)F(\zeta,\xi) - \exp(-\pi\zeta^2/\xi)G(\tfrac{1}{2}\zeta;\lambda;\xi)$$

and

$$H_0(\zeta;\lambda;\xi) = H(\zeta;\lambda;\xi)/H(1;\tfrac{1}{2};\xi)$$

so that $H_0(\zeta;\lambda;\xi)$ is a scaled two-particle distribution function. We plot contours of $H_0(\zeta;\lambda;\xi)$ in Figs. 2a, b, c, d.

At small ξ, the particles clearly lie in ridges normal to the x axis with very little correlation between the particles in each ridge. Near $\xi = 2$ the particles show some tendency to take up an alternating structure in the ζ,λ plane at $(0,0), (1,\frac{1}{2}), (2,0), \ldots,$ a structure reminiscent of a solid. The strong peak at $(1,\frac{1}{2})$ for $\xi = 2$ is a particularly good example of this

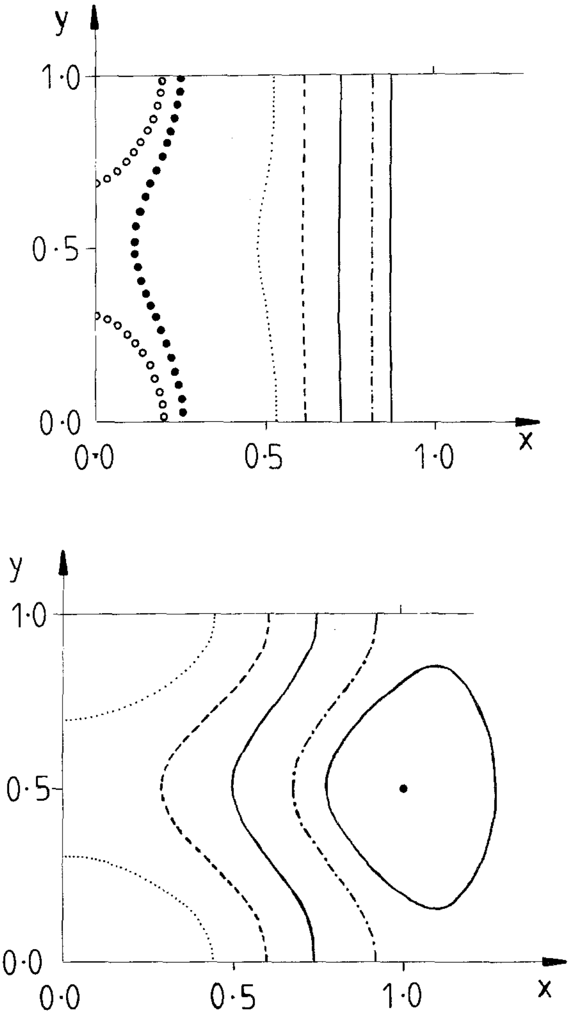

Fig. 2. Plots of contours of $H_0(\zeta, \lambda, \xi)$ from left to right. OOOOO: contour $H_0(\zeta, \lambda, \xi) = 0.01$; ●●●●●: contour $H_0(\zeta, \lambda, \xi) = 0.02$; ········: contour $H_0(\zeta, \lambda, \xi) = 0.2$; – – – –: contour $H_0(\zeta, \lambda, \xi) = 0.4$; ———: contour $H_0(\zeta, \lambda, \xi) = 0.6$; –·–·–·–: contour $H_0(\zeta, \lambda, \xi) = 0.8$; ———: contour $H_0(\zeta, \lambda, \xi) = 0.9$. a: $\xi = 1.0$; b: $\xi = 2.0$; c: $\xi = 2\sqrt{3}$; d: $\xi = 4$.

alternating structure. At larger ξ, the particles become too crowded to sustain such an ordered structure. A cross section $H_0(\xi; \frac{1}{2}; \xi)$ is plotted in Fig. 3 and confirms this picture.

The consequences of these results for the theory of the simulation of ionic systems in general are not clear. It is certainly true that the layered

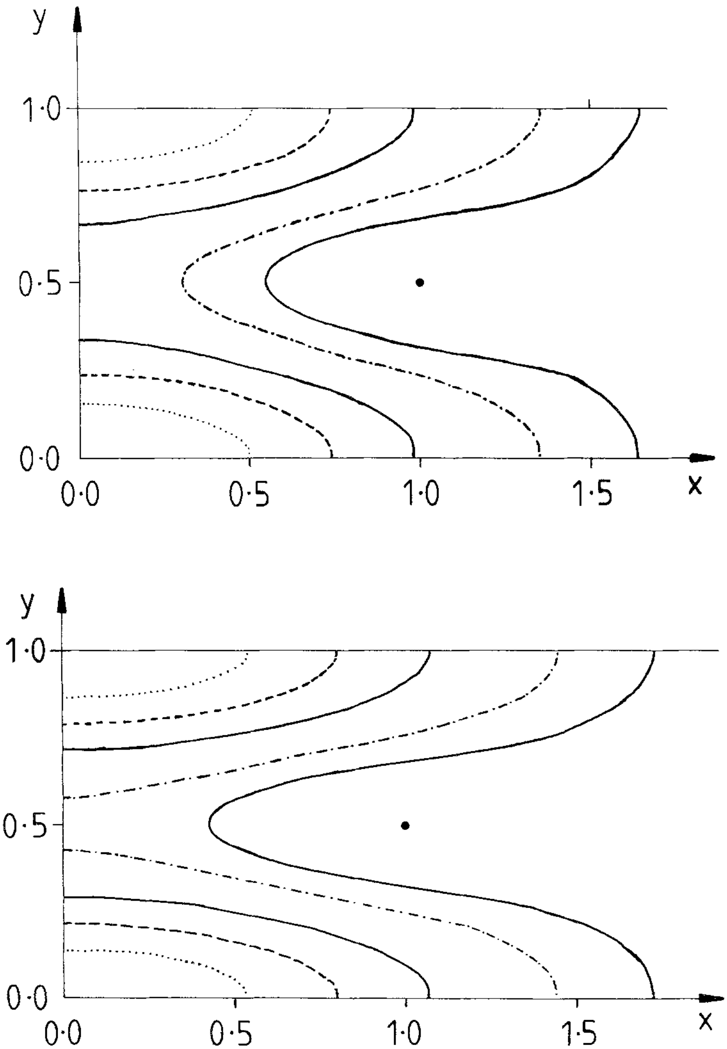

Fig. 2. Continued.

structures have been observed in Monte Carlo simulations of systems of hard spheres with embedded point charges.[13-15] It is also tempting to identify some of the problems encountered in early simulations of charged systems[16,17] with similar effects.

Finally, a recent paper of Gruber and Martin[18] shows that $\mathscr{L}^1$-clustering equilibrium states of classical systems of point particles are translationally invariant and specifically notes the case of a one-component

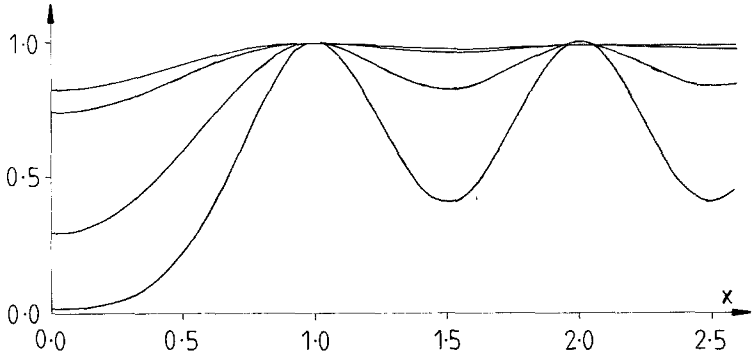

Fig. 3. Plots of $H_0(\zeta, 1/2, \xi)$ from bottom to top: $\xi = 1.0$, $\xi = 2.0$, $\xi = 2\sqrt{3}$, $\xi = 4.0$.

plasma in dimension $d \geqslant 2$. We note here that the proof for the two-dimensional one-component plasma requires that the interparticle force tend to zero at large separation. Here, as $|x_j - x_k| \to \infty$, the x component of this force tends to $-\pi\,\mathrm{sgn}(|x_j - x_k|)/W$. Thus the theorem is not applicable to this system.

REFERENCES

1. B. Jancovici, *Phys. Rev. Lett.* **46**:386 (1981).
2. B. Jancovici, *J. Stat. Phys.* **28**:43 (1981).
3. B. Jancovici, *J. Stat. Phys.* **29**:263 (1982).
4. E. R. Smith, *Phys. Rev. A* **24**:2851 (1981).
5. E. R. Smith, *J. Phys. A. Math. Gen.* **15**:1271 (1982).
6. P. J. Forrester and E. R. Smith, *J. Phys. A. Math. Gen.* **15**:3861 (1982).
7. P. J. Forrester, B. Jancovici, and E. R. Smith, *J. Stat. Phys.*, to appear.
8. Ch. Gruber, J. L. Lebowitz, and Ph. A. Martin, *J. Chem. Phys.* **75**:944 (1981).
9. L. Blum, Ch. Gruber, J. L. Lebowitz, and Ph. A. Martin, *Phys. Rev. Lett.* **48**:1769 (1982).
10. L. Blum, D. Henderson, J. L. Lebowitz, Ch. Gruber, and Ph. A. Martin, *J. Chem. Phys.* **75**:5974 (1981).
11. Ph. Choquard, *Helv. Phys. Acta* **54**:332 (1981).
12. H. Kunz, *Ann. Phys.* (N.Y.) **85**:303 (1974).
13. J. Valleau, private communication.
14. C. S. Hoskins and E. R. Smith, *Mol. Phys.* **41**:243 (1980).
15. D. Adams, *Chem. Phys. Lett.* **62**:329 (1979).
16. S. G. Brush, H. L. Sahlin, and E. J. Teller, *J. Chem. Phys.* **45**:2102 (1966).
17. L. V. Woodcock and K. Singer, *Trans. Faraday Soc.* **67**:12 (1971).
18. Ch. Gruber and Ph. A. Martin, *Phys. Rev. Lett.* **45**:853 (1980).