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On the thermodynamics of the two-dimensional jellium

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Abstract. We consider the two-dimensional classical jellium in a circular domain. Using a careful extrapolation method of the exact results for systems with a small number of particles ($N = 1, 2, 3, 4$), we obtain an estimate of the free-energy density and the kinetic pressure in the thermodynamic limit for some discrete values of the plasma parameter $2 \leq \gamma \leq 14$. An ansatz for the free-energy density is then constructed which is in good agreement with the theoretical estimation and the numerical results of a recent Monte Carlo simulation of the system. A similar agreement is obtained for the kinetic or virial pressure.

1. Introduction

The two-dimensional jellium (two-dimensional one-component plasma) has received much attention lately. In a theoretical context, the motivation to investigate the properties of such a system is related to one of the fundamental questions in statistical mechanics of charged particles, namely if classical statistical mechanics may describe a crystalline state (or more generally an ordered state) in a model with long-range Coulomb forces at sufficiently low temperatures. In a similar two-dimensional model, recent computer experiments indicate the existence of a solid phase characterised by a directional long-range order and an approximate long-range positional order in the practical case of a finite system (Gann *et al* 1979); moreover, the three-dimensional jellium is 'realised' and investigated experimentally (Malmberg and O'Neil 1977, Prasad and O'Neil 1979).

The classical model consists of N charged particles (electrons of charge $-e$) immersed in a uniform neutralising background of positive charge density $+\rho e = eN/|\Lambda|$, in a domain Λ. The microscopic interaction between two point charges is the long-range genuine two-dimensional Coulomb potential given by $\varphi(|\boldsymbol{x}|) = -e^2 \ln|\boldsymbol{x}|$ where $|\boldsymbol{x}|$ is the distance between the two interacting charges. The thermodynamic state of this system is characterised essentially by the two-dimensional plasma parameter $\gamma = \beta e^2$ ($\beta = 1/kT$), and the free-energy density in the thermodynamic limit $\Lambda \nearrow \mathbb{R}^2$ for Λ of reasonable shape exists (Sari and Merlini 1976); moreover, the ground state consists of a configuration in which the electrons form a triangular lattice (Sari *et al* 1976). Recently it has been shown that in such a system shape-dependent properties exist (Choquard 1978); for example, if one computes the particle density

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at the wall (boundary of Λ) then, as Λ becomes large, this approaches a value smaller than the mean density ρ, called the kinetic or virial pressure p_v; $p_v \neq p_{th}$ where p_{th} is the thermal pressure, known to become negative at moderately high values of the plasma parameter. The model has also been treated recently in various truncation schemes of the BBGKY equilibrium hierarchy and the solution reveals a very simple form of the free-energy density and correlation energy as a function of γ (Calinon *et al* 1979, Bakshi *et al* 1979, 1981), which is in good agreement with the numerical result of a Monte Carlo simulation of the system (Calinon and Choquard 1979, see also Choquard *et al* 1980b). A non-analytic behaviour of the thermodynamics has, at the present time, not been discovered. Since the free energy is shape and boundary independent (Albeverio *et al* 1982), to investigate the thermodynamics it is sufficient to treat the model in an open circular domain Λ of radius $R = (N/\pi\rho)^{1/2}$.

In this work we present some preliminary analytical results on the thermodynamic and kinetic pressure up to moderately high values of the plasma parameter γ. We first define the model and recall some known results concerning the exact thermodynamics, particle density, and pair correlation function for the special value $\gamma = 2$ and then check an important sum rule. We then compute the partition function of the model with a small number of particles in terms of small polynomials up to $\gamma = 12$ (§ 2), and we obtain new rigorous upper and lower bounds of the free energy in the thermodynamic limit (§ 3). Finally a careful analysis of the way in which the thermodynamic limit is approached at $\gamma = 2$ together with the exact computations for $N = 1$, 2, 3, 4 allow us to obtain an estimate of the free energy at $\gamma \geq 2$ up to $\gamma = 14$ which is in good agreement with a theoretical ansatz (§ 4) and the result of a computer experiment of the system; a similar treatment allows an estimate for the kinetic pressure in good agreement with the results of a Monte Carlo simulation of the system (§ 5). We then briefly give our conclusions (§ 6).

2. Definition of the model and some exact computations

The model we consider (two-dimensional one-component plasma = 2D OCP) is made up of N point charges of charge $-e$ immersed in a homogeneous neutralising charge background of charge density $+\rho e$, in a domain Λ of volume $|\Lambda| = \pi R^2$ (we restrict here to circular domains of radius R and we assume charge neutrality: $\rho = N/|\Lambda|$). The microscopic interaction between two point charges is the two-dimensional long-range Coulomb potential given by $\gamma(\boldsymbol{x}_1, \boldsymbol{x}_2) = -e^2 \ln(|\boldsymbol{x}_1 - \boldsymbol{x}_2|)$. The Hamiltonian then reads (Sari *et al* 1976)

$$H = H_{pp} + H_{pb} + H_{bb} = \tfrac{1}{2}e^2\pi\rho \sum_{i=1}^{N} \boldsymbol{x}_i^2 - e^2 \sum_{\substack{i<j\\ i=1}}^{N} \ln(|\boldsymbol{x}_i - \boldsymbol{x}_j|) + e^2(\tfrac{1}{2}N^2 \ln R - \tfrac{3}{8}N^2)$$

where p, b stand for particles and background respectively and $\{\boldsymbol{x}_i\}$ are the positions of the N point charges.

2.1. Partition function

By definition we have

$$Q_\gamma(N) = \frac{1}{N!} \int_{\Lambda^N} d\{x\}\, e^{-\beta H} \tag{1}$$

where $d\{x\}=\prod_{i=1}^{N} d^2x_i$. With the change of variables: $\pi\rho x_i^2 = z_i^2$, we obtain

$$Q_\gamma(N)=\frac{|\Lambda|^N}{N!}\frac{e^{\gamma NB}}{N^N}\exp[\gamma(\tfrac{3}{8})N(N-1)-\tfrac{1}{4}N^2\ln N)]\int_0^N\prod_{i=1}^N dz_i^2$$
$$\times\exp\left(-\tfrac{1}{2}\gamma\sum_{i=1}^N z_i^2\right)\alpha(\{|z_i|\}) \qquad (2)$$

where $\gamma=\beta e^2$ is the two-dimensional plasma parameter, $\beta=1/kT$ and $-B=-(\frac{1}{4}\ln\pi\rho+\frac{3}{8})$ is the H-stability bound (Sari and Merlini 1976);

$$\alpha(\{z_i|\})=\frac{1}{(2\pi)^N}\int d\varphi_1\ldots d\varphi_N\prod_{i<j}\||z_i-z_j|^\gamma$$

is a homogeneous polynomial of degree $\frac{1}{2}\gamma N(N-1)$, symmetric in the z_i obtained after integration over the angles $\{\varphi_i\}$. The free energy per particle is given by

$$-\beta f_\gamma=(1/N)\ln Q_\gamma(N)=-f_\gamma/e^2.$$

For futher use, it is useful to consider the excess free energy with respect to the H-stability bound $-B$ and the perfect gas limit, i.e.

$$\bar{f}_\gamma=f_\gamma+B\gamma+\frac{1}{N}\ln\left(\frac{|\Lambda|^N}{N^N e^{-N}}\right)$$
$$=\gamma[\tfrac{1}{4}N\ln N-\tfrac{3}{8}(N-1)]+1-\frac{1}{N}\ln\int_0^N\prod_{i=1}^N dz_i^2\exp\left(-\tfrac{1}{2}\gamma\sum_{i=1}^N z_i^2\right)\frac{\alpha(\{|z_i|\})}{N!} \qquad (3)$$

and

$$\bar{\bar{f}}_\gamma=f_\gamma+B\gamma+\frac{1}{N}\ln\left(\frac{|\Lambda|^N}{N!}\right)=\bar{f}_\gamma+\frac{1}{N}\ln\left(\frac{N^N e^{-N}}{N!}\right)=\bar{f}_\gamma+\Delta_N.$$

As $N\to\infty$, $\bar{f}_\gamma=\bar{\bar{f}}_\gamma$. The reason for considering $\bar{\bar{f}}_\gamma$ and $\bar{f}_\gamma$ will become clear later on in § 4, where we carry out our analytical computations for very small N. Some exact computations can be done for the special value $\gamma=2$ by using an identity first considered by Mehta (1967) and used recently to obtain new interesting results at the same value of γ (Deutsch *et al* 1979, Alastuey and Jancovici 1981, Jancovici 1981a, b), i.e.

$$\alpha(\{|z_i|\})_{\gamma=2}=\int_0^{2\pi}\frac{d\varphi_1\ldots d\varphi_N}{(2\pi)^N}\prod_{\substack{i<j\\ i=1}}^N|z_i-z_j|^2=N!\prod_{i=1}^N|z_i|^{2(i-1)}. \qquad (4)$$

Notice that for the thermodynamic limit of the free energy, it is justified to extend the upper limit of integration in (3) from N to ∞ (Alastuey and Jancovici 1981). Thus:

$$\bar{f}_{\gamma=2}=\bar{\bar{f}}_{\gamma=2}=\lim_{N\to\infty}2[\tfrac{1}{4}N\ln N-\tfrac{3}{8}(N-1)]+1-\frac{1}{N}\ln\int_0^\infty\prod_{i=1}d|z_i|^2$$
$$\times\exp\left(-\sum_i|z_i|^2\right)|z_i|^{2(i-1)}. \qquad (5)$$

The last term yields exactly the Vandermonde determinant, which for large N is given

(Schwarz 1965) by

$$\ln V_N = \tfrac{1}{2}N^2 \ln N - \tfrac{3}{4}N^2 + \tfrac{1}{2}N \ln 2\pi - \tfrac{1}{12} \ln N, \tag{6}$$

so that

$$\bar{f}_{\gamma=2} = \tfrac{7}{4} - \tfrac{1}{2} \ln 2\pi = 0.831\,059\,4.$$

The above known exact value will be used later on, in the construction of new upper and lower bounds for the free energy for $\gamma \neq 2$ and for an analytical ansatz for f_γ as a function of γ.

2.2. *One-body correlation function*

From the definition

$$f_1(\boldsymbol{x}_1) = \frac{N!}{(N-1)!} \frac{\int \mathrm{d}_2 \ldots \mathrm{d}_N \, \mathrm{e}^{-\beta H}}{\int \mathrm{d}_1 \ldots \mathrm{d}_N \, \mathrm{e}^{-\beta H}} \tag{7}$$

and since $f_1(x_1)$ is rotational invariant we have

$$f_1(\boldsymbol{x}_1) = \rho N \frac{\int_0^N \Pi_{i=2}^N \, \mathrm{d}z_i^2 \, \exp(-\tfrac{1}{2}\gamma \, \Sigma_i z_i^2)\alpha(\{z_i\})}{\int_0^N \Pi_{i=1}^N \, \mathrm{d}z_i^2 \, \exp(-\tfrac{1}{2}\gamma \, \Sigma_i z_i^2)\alpha(\{z_i\})}. \tag{8}$$

For $\gamma = 2$

$$f_1(z) = \rho \sum_{i=1}^{N} \frac{z^{2(i-1)} \exp(-z^2)}{\int_0^N \mathrm{d}z^2 \exp(-z^2) z^{2(i-1)}}. \tag{9}$$

For $z^2 \ll N$, the upper limit of integration in the denominator can be extended to ∞ as for the computation of the free energy so that (Mehta 1967)

$$f_1(z) = \rho \sum_{i=1}^{\infty} \exp(-z^2) \frac{z^{2(i-1)}}{(i-1)!} = \rho. \tag{10}$$

Thus, for $\gamma = 2$ the state is homogeneous.

It should be remarked that the situation is different if one computes the density $f_1(z)$ for $z^2 = N$, i.e. at the boundary of Λ, as $N \to \infty$.

The computation is of interest since the density at the wall, normalised to ρ, is the kinetic or virial pressure (Calinon and Choquard 1979, Choquard *et al* 1980a, b, Calinon and Merlini 1980). We obtain

$$\frac{f_1(N)}{\rho} = \left(\frac{\beta p_{\mathrm{v}}}{\rho}\right)_{\gamma=2} = \sum_{i=1}^{N-1} \frac{\mathrm{e}^{-N} N^i}{\int_0^N \mathrm{d}z^2 \exp(-z^2) z^{2i}}. \tag{11}$$

Recalling that the thermal pressure (Hauge and Hemmer 1971) is rigorously given by (Sari and Merlini 1976)

$$\beta p_{\mathrm{th}} = -\rho^2 (\partial/\partial\rho)(-f_\gamma/\rho) = \rho(1 - \tfrac{1}{4}\gamma) \tag{12}$$

we see that *if* the limit of integration in (11) is extended up to ∞, then

$$\lim_{N\to\infty} \sum_{i=1}^{N-1} \frac{\mathrm{e}^{-N} N^i}{i!} = \tfrac{1}{2} = \frac{\beta p_{\mathrm{th}}}{\rho}(\gamma = 2). \tag{13}$$

From the above $\tfrac{1}{2} \leq (\beta p_{\mathrm{v}}/\rho)_{\gamma=2} \leq 1$. A linear extrapolation of $f_1(N)$ for $\gamma = 2$ as function of $x = 1/N$, up to $N = 10$ (see § 5), gives the estimate $(\beta p_{\mathrm{v}}/\rho)_{\gamma=2} \cong 0.684$ which is about 30% greater than the thermal pressure.

2.3. Two-body correlation function

It is defined by

$$f_2(\boldsymbol{x}_1, \boldsymbol{x}_2) = \frac{N!}{(N-2)!} \frac{\int d_3 \ldots d_N \, e^{-\beta H}}{\int d_1 \, d_2 \ldots d_N \, e^{-\beta H}}. \tag{14}$$

For $\gamma = 2$ it is known (Mehta 1967), that the net correlation function g, i.e. $f_2 - \rho^2 = g\rho^2$, is Gaussian-like, i.e.

$$g(|\boldsymbol{x}_1 - \boldsymbol{x}_2|) = -\exp[-\pi\rho(\boldsymbol{x}_1 - \boldsymbol{x}_2)^2]. \tag{15}$$

The correlation energy is given by (Jancovici 1981a, b)

$$(1/\beta)E_c(\gamma = 2) = \tfrac{1}{2} \int d^2\boldsymbol{r} \, \rho g(\boldsymbol{r}) \ln r = \langle H \rangle / N = -B + \tfrac{3}{8} - \tfrac{1}{4}c \tag{16}$$

where $c = 0.577216$ is the Euler constant. Thus

$$E_{\gamma=2} = \langle H \rangle / N + B = \tfrac{3}{8} - \tfrac{1}{4}c = 0.230696. \tag{17}$$

Again, the above exact value will be useful in constructing an analytical expression or 'ansatz' for f_γ as function of γ. We now check that the compressibility sum rule is satisfied at $\gamma = 2$.

If we denote by $\varepsilon(\xi, 0)$, the static long-wavelength dielectric response function in the reduced variable $\xi = |\boldsymbol{K}|/K_D$, $K_D = (2\pi\gamma\rho)^{1/2}$, the sum rule (Golden and Merlini 1977) states that

$$\lim_{\xi \to 0} (\varepsilon(\xi_1 0) - 1)\xi^2 = \frac{1}{(\beta p_{\text{th}}/\rho)} = \frac{1}{(1 - \gamma/4)} \tag{18}$$

with the help of equation (12).

Let $S(\boldsymbol{K}) = g(\boldsymbol{K}) + 1$ be the Fourier transform of the structure factor. By applying the linear fluctuation dissipation theorem

$$S(\xi) = \xi^2(1 - 1/\varepsilon(\xi_1 0)) \tag{19}$$

to (18) we obtain

$$\lim_{\xi \to 0} \frac{S(\xi)}{1 - S(\xi)/\xi^2} = \frac{1}{(1 - \gamma/4)}. \tag{20}$$

Since $g(\boldsymbol{K}) = \bar{g}(\xi) = \exp(-\xi^2)$ at $\gamma = 2$ from (20) we obtain

$$\left(\frac{\beta p_{\text{th}}}{\rho}\right)_{\gamma=2} = \lim \frac{\xi^2 - S(\xi)}{\xi^2 S(\xi)} = \frac{\xi^4/2}{\xi^2} = \frac{1}{2}$$

which proves that the rule is satisfied at $\gamma = 2$. It has been shown recently that the above rule is satisfied for each value of the plasma parameter in the convolution approximation (Bakshi *et al* 1981).

It should be remarked that exact computations for $\gamma \neq 2$ as far as we know are at the present time still lacking: in fact the identity given by (4) holds only for $\gamma = 2$ and for $\gamma \neq 2$ integration over the angles $\{\varphi_i\}$ yields more complicated polynomials in the z_i. Our analytical results for small N follow from the computations of the $\alpha(\{z_i\})$ for

$N=2$ and $\gamma=2, 4, 6, \ldots, 12$ given below:

	$\alpha(z_1, z_2)$
$\gamma=2$	$z_1^2+z_2^2$
$\gamma=4$	$z_1^2+z_4^4+4z_1^2z_2^2$
$\gamma=6$	$z_1^6+z_2^6+9z_1^4z_2^2+9z_1^2z_2^4$
$\gamma=8$	$z_1^8+z_2^8+36z_1^4z_2^4+16z_1^6z_2^2+16z_1^2z_2^6$
$\gamma=10$	$z_1^{10}+z_2^{10}+25z_1^8z_2^2+25z_1^2z_2^8+100z_1^4z_2^6$
$\gamma=12$	$z_1^{12}+z_2^{12}+36z_1^{10}z_2^2+36z_1^2z_2^{10}+225z_1^8z_2^4+225z_1^4z_2^8+400z_1^6z_2^6.$

In § 4 we will compute exactly the free energy for $N=1, 2, 3, 4$ up to $\gamma=14$, using the above polynomials; extrapolation of the results will then yield, up to $\gamma=14$, an approximated value for f_γ in the thermodynamic limit in good agreement with the result of a Monte Carlo simulation of the system and a theoretical ansatz.

3. Upper and lower bounds to the free energy

In order to situate and compare our analytical results for small N and our extrapolation (see §§ 4 and 5), with the results of a Monte Carlo simulation of the system with $N=37$ particles (Calinon and Choquard 1979, see also Choquard *et al* 1980b), we use the exact results for $\gamma=2$ and derive some refined bounds on the free energy which improve those previously given (Sari and Merlini 1976). The bounds are obtained by means of the Jensen inequality and the H-stability bound for the energy. With

$$f_\gamma=-(1/N)\ln Q_\gamma(N)+B\gamma+(1/\rho)(1-\ln\rho)$$

and

$$E_\gamma=(1/N)\langle H\rangle_\gamma+B$$

the Jensen inequality yields

$$Q_\gamma=\frac{1}{N!}\int d\{x\}\,e^{-\gamma H}=\frac{1}{N!}\int d\{x\}\,e^{-2H}\,e^{-(\gamma-2)H}\geqslant Q_2\exp[-(\gamma-2)\langle H\rangle_2]$$

so that

$$\bar{f}_\gamma\leqslant\bar{f}_2+(\gamma-2)E_2.$$

Since $\bar{f}_2=0.8310592$ and $E_2=0.230696$ a rigorous upper bound is given by

$$\bar{f}_\gamma\leqslant 0.831\,059\,2+(\gamma-2)0.230\,696. \tag{21}$$

A lower bound is obtained in the same way by using the H-stability bound:

$$Q_\gamma=\frac{1}{N!}\int d\{x\}\,e^{-\gamma H}=\frac{1}{N!}\int d\{x\}\,e^{-2H}\,e^{-(\gamma-2)H}.$$

Since $H\geqslant-N(B-\varepsilon)$, then

$$Q_\gamma\leqslant\frac{1}{N!}\int d\{x\}\,e^{-2H}\exp[(\gamma-2)(B-\varepsilon)N]$$

and thus

$$\bar{f}_\gamma \geq \bar{f}_2 + (\gamma - 2)\varepsilon. \tag{22}$$

Notice that $-N(B-\varepsilon)$ is the minimum value of the energy for $N>1$. ε has been found to satisfy $0.000\,62 \leq \varepsilon < 0.017$ for for the perfect triangular lattice configuration (Sari *et al* 1976, Alastuey and Jancovici 1981). A configuration with lower energy has not yet been found. Thus

$$\bar{f}_\gamma \geq 0.831\,059\,2 + (\gamma - 2)0.000\,62 \tag{23}$$

where for ε we have taken the value $\varepsilon = 0.000\,62$.

4. Exact computation of the free energy density for small N and extrapolation

We now compute exactly the free energy density for very small N, i.e. $N = 1, 2, 3, 4$ and up to moderately high values of the plasma parameter $\gamma = (1/kT)e^2 \leq 14$. As noted in § 2, we assume that for the computation of $\bar{f}_\gamma$ in (3) the upper limit of integration for the z_i can be extended from N to ∞. This was justified for $\gamma = 2$ (Alastuey and Jancovici 1981) and is expected to hold for $\gamma > 2$, in view of the presence of Gaussian terms proportional to γ in the integral; this was checked explicitly for $N = 1$ and $N = 2$. Nevertheless, in doing so we have no proof that $\bar{f}_\gamma$ calculated with (3) is more than a rigorous lower bound to the exact free energy for $\gamma \neq 2$.

4.1. *Computation for small N*

The computation for $N = 1$ is immediate and we get

$$\bar{f}_\gamma = \ln \tfrac{1}{2}\gamma + 1 \qquad \bar{\bar{f}}_\gamma = \ln \tfrac{1}{2}\gamma. \tag{24}$$

The exact computation of the free energy for $N = 1$, where the upper limit of integration is $N = 1$, gives

$$\bar{f}_\gamma = \ln \tfrac{1}{2}\gamma + 1 - \ln(1 - e^{-\gamma/2}) \qquad \bar{\bar{f}}_\gamma = \ln \tfrac{1}{2}\gamma - \ln(1 - e^{-\gamma/2}).$$

For $\gamma > 6$, $e^{-\gamma/2} < 0.06$ and the two results are in good agreement.

The computation for $N = 2$ is easily obtained by means of the variable transformation: $y_1 = (\gamma/4)^{1/2}(z_1 + z_2)$, $y_2 = (\gamma/4)^{1/2}(z_1 - z_2)$, which gives

$$\bar{f}_\gamma = \gamma(\tfrac{1}{2}\ln 2 - \tfrac{3}{8}) + 1 - \frac{1}{2}\ln\left(\frac{(\gamma/2)!2^{\gamma-1}}{\gamma^{\gamma/2}(\gamma/2)^2}\right) \tag{25}$$

$$\bar{\bar{f}}_\gamma = \bar{f}_\gamma - \tfrac{1}{2}(2 - \ln 2). \tag{26}$$

As before, it can be checked explicitly that the error due to the extension of the upper limit of integration from $N = 2$ to ∞ is small for every γ as in the case $N = 1$.

For $N = 3$ the computation is not as easy as for $N = 2$ (see Mehta 1967, appendix A for a similar computation in the one-dimensional case). Nevertheless, following Mehta and using a variable transformation, the computation can be carried out as follows. Introduce

$$y_1 = \left(\frac{\gamma}{4}\right)^{1/2}(z_1 - z_2) \qquad y_2 = \left(\frac{\gamma}{12}\right)^{1/2}(z_1 + z_2 - 2z_3) \qquad y_3 = \left(\frac{\gamma}{6}\right)^{1/2}(z_1 + z_2 + z_3). \tag{27}$$

We then obtain

$$\bar{f}_\gamma = \gamma \tfrac{3}{4}(\ln 3 - 1) + 1$$
$$-\frac{1}{3}\ln\left(\frac{\int_0^\infty \int_0^\infty \mathrm{d}y_1^2\, \mathrm{d}y_2^2 \int_0^{2\pi} (\mathrm{d}\varphi/2\pi) y_1^\gamma \exp(-y_1^2 - y_2^2)(y_1^4 + y_2^4 - 6y_1^2 y_2^2 \cos\varphi)^{\gamma/2}}{3!\, 2^{\gamma/2}(\gamma/2)^{3/2\gamma}}\right).$$

With the change of variables $y_1^2 = \bar{z}_1^2$, $3y_2^2 = \bar{z}_2^2$, we see that the computation can be carried out with the help of the values of $\alpha(\{z_i\})$ for $N = 2$ given in § 2. The results for $N = 1, 2, 3$ and up to $\gamma = 14$ are given in table 1 below.

Table 1.

	γ	$\bar{\bar{f}}_\gamma$	$\bar{f}_\gamma$
$N = 1$	2	0	1
	4	0.693 15	1.693 15
	6	1.098 61	2.098 61
	8	1.386 4	2.386 4
	10	1.609 44	2.609 44
	12	1.791 76	2.791 76
	14	1.945 91	2.945 91
$N = 2$	2	0.289 72	0.943 14
	4	0.926 01	1.579 44
	6	1.333 51	1.986 94
	8	1.649 29	2.302 72
	10	1.915 30	2.568 72
	12	2.150 00	2.803 42
	14	2.363 17	3.016 60
$N = 3$	2	0.418 22	0.916 86
	4	1.017 987	1.516 62
	6	1.404 56	1.903 20
	8	1.698 90	2.197 54
	10	1.939 94	2.438 58
	12	2.146 04	2.644 68
	14	2.327 57	2.826 21

4.2. Extrapolation method

We first show that the knowledge of the free energy for small N, $N \leq 5$ at $\gamma = 2$ is very useful to obtain an extrapolated result for the free energy density, which is a very good approximation to the exact free energy in the thermodynamic limit given by (6).

For $\gamma = 2$ the computation of the sequence $\bar{f}_\gamma$, $\bar{\bar{f}}_\gamma$ up to $N = 5$ is easy and we obtain the sequence given in table 2.

Now, the method of extrapolation for $\bar{f}_\gamma$, $\bar{\bar{f}}_\gamma$ to large N, which we will adopt later for $\gamma \geq 2$, is suggested by the exact asymptotic behaviour of the Vandermonde determinant considered in § 2. In fact from (5), we have

$$\bar{f}_{\gamma=2} = 2[\tfrac{1}{4}N \ln N - \tfrac{3}{8}(N-1)] + 1 - (1/N)\ln\left(\prod_{K=1}^{N-1} K!\right).$$

Table 2.

N	$\bar{\bar{f}}_{\gamma=2}$	$\bar{f}_{\gamma=2}$
1	0	1
2	0.289 725	0.931 5
3	0.418 214	0.916 86
4	0.493 153	0.901 37
5	0.542 946	0.891 00

Introducing the variable $x = 1/N$, and using the formula $K! = (2\pi)^{1/2} \exp[(K+\frac{1}{2})\ln K - K + 1/12K - 1/300K^3]$ for every K and remembering that by definition the Euler constant $c = 0.577216$ is given by

$$c = \lim_{K\to\infty} \sum_{n=1}^{K} (1/n - \ln n)$$

it can be shown that the asymptotic limit is approached as

$$\bar{f}_{\gamma=2}(x) = \bar{f}_{\gamma=2}(0) + \tfrac{1}{12}x \ln x + x(\tfrac{1}{8}\ln 2\pi - \tfrac{1}{24}(c+1)) + \tfrac{1}{48}x^2 + \ldots$$

$$\bar{\bar{f}}_{\gamma=2}(x) = \bar{\bar{f}}_{\gamma=2}(0) + \tfrac{1}{2}x \ln x - \tfrac{1}{2}x \ln 2\pi - \tfrac{1}{12}x^2 + \ldots.$$

Our analysis for $\gamma = 2$ suggests to extrapolate the values of $\bar{f}_\gamma$ and $\bar{\bar{f}}_\gamma$ to large N and arbitrary γ by the ansatz

$$\bar{f}_\gamma(x) = \bar{f}_\gamma(0) + ax + bx \ln x + cx^2 + \ldots \tag{28}$$

where a, b, c depend on γ (we believe that (28) above is not restricted to the particular value $\gamma = 2$). For $\gamma = 2$, using the results for $N = 1, 2, 3$ and putting $c = 0$, the above expression yields the asymptotic values $\bar{f}_{\gamma=2}(0) = 0.833\,28$ and $\bar{\bar{f}}_{\gamma=2}(0) = 0.810\,128$; using in the same way the results for $N = 2, 3, 4$ we obtain $\bar{f}_{\gamma=2}(0) = 0.831\,99$ and $\bar{\bar{f}}_{\gamma=2}(0) = 0.822\,51$. On the other hand, using the results for $N = 3, 4, 5$ we obtain the values $\bar{f}_{\gamma=2}(0) = 0.831$ and $\bar{\bar{f}}_{\gamma=2}(0) = 0.825$, which are in excellent agreement (up to 5×10^{-3}) with the exact value in the thermodynamic limit $\bar{f}_{\gamma=2} = 0.831\,059\,4$ given by (6).

Using the above method of extrapolation, we have first computed the free energy up to $\gamma = 10$ using the results for $N = 1, 2, 3$. The values are given in table 3.

Table 3. Free energy for $\gamma = 2, 4, 6, 8, 10$.

γ	$\bar{f}_\gamma$	$\bar{\bar{f}}_\gamma$
2	0.833 273	0.810 177
4	1.262 485	1.285 583
6	1.486 23	1.538 906
8	1.637 015	1.660 11
10	1.662 073	1.685 17

In analogy with the results obtained in a refined truncation scheme of the BBGKY hierarchy (Calinon *et al* 1979) and in a recent Monte Carlo simulation of the system (Calinon and Choquard 1979, see also Choquard *et al* 1980b), we consider an analytical ansatz for the free energy density given by

$$f_\gamma = a\gamma - b\gamma \ln\left(\frac{\gamma}{\gamma + c}\right) + bc \ln\left(\frac{\gamma + c}{c}\right). \tag{29}$$

From (29) the correlation energy and the excess specific heat take the simple form

$$E_\gamma = a - b \ln[\gamma/(\gamma + c)] \tag{30}$$

$$c_\nu = bc[\gamma/(\gamma + c)]. \tag{31}$$

To find the values of a, b, c, in (29) we use the exact results for $f_{\gamma=2}$, $E_{\gamma=2}$ and we assume that a is the lowest value of the energy at $T = 0$, i.e. that of the perfect triangular crystalline configuration given in § 2, i.e. $a = \frac{3}{8} - 0.374\,38 = 0.000\,62$.

For this purpose we may put $a = 0$; we then get $c = 3.3$ and $b = 0.236\,715\,5$. Our results are presented in figure 1 where we plot the free energy f_γ/γ given by the analytical ansatz (29), the average $\frac{1}{2}(\bar{f}_\gamma + \bar{\bar{f}}_\gamma)$ given by our method of extrapolation and the theoretical rigorous upper and lower bounds given by (21) and (23). The concave function of γ given by (29) appears as a correct attractor to the results of our extrapolation method. It is expected that a computer computation of $\bar{f}_\gamma$ up to $\gamma = 200$ and up to $N = 6$ will yield the thermodynamic free energy exact up to 10^{-5} and more conclusions will be obtained about the thermodynamics of the two-dimensional OCP (Johannesen and Merlini 1982). To conclude, we present the method of computation for $N > 3$ and check the usefulness of the approach using the more realistic results for $N = 2, 3, 4$ particles.

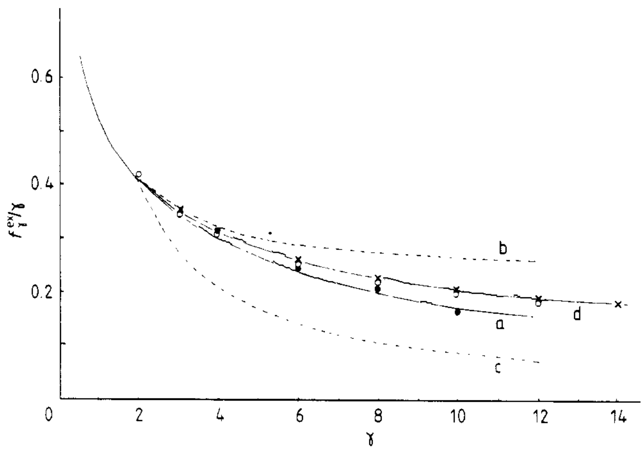

Figure 1. The free energy density as function of γ following the ansatz given by (29) (curve a), the rigorous upper and lower bounds (b and c) from (23) and (21); the full circles are the results with $N = 1, 2, 3$ from table 3 and the crosses are our results with $N = 2, 3, 4$ from table 5. Curve d is the ansatz (29) with a, b, c determined with the values of $f = (\bar{f}_\gamma + \bar{\bar{f}}_\gamma)/2\gamma$ at $\gamma = 14$, $\gamma = 10$ and $\gamma = 6$. The open circles are the results of computer experiments (Calinon and Choquard 1979, see also Choquard 1980b).

4.3. *Method of computation for $N > 3$*

The variable transformation given by (27) may in principle be generalised to the case $N > 3$. This is of interest for further numerical computations, since the number of variables may be reduced. Let us now consider the case $N=4$. Then instead of (27) we have

$$y_1=(\gamma/4)^{1/2}(z_1-z_2) \qquad y_2=(\gamma/12)^{1/2}(z_1+z_2-2z_3)$$
$$y_3=(\gamma/24)^{1/2}(z_1+z_2+z_3-3z_4) \qquad y_4=(\gamma/8)^{1/2}(z_1+z_2+z_3+z_4). \tag{32}$$

Nevertheless, we found it to be more convenient to consider the similar transformation given by

$$y_1=(\gamma/8)^{1/2}(z_1-z_2-z_3+z_4) \qquad y_2=(\gamma/8)^{1/2}(z_1-z_2+z_3-z_4)$$
$$y_3=(\gamma/8)^{1/2}(z_1+z_2-z_3-z_4) \qquad y_4=(\gamma/8)^{1/2}(z_1+z_2+z_3+z_4). \tag{33}$$

From above $\frac{1}{2}\gamma\sum_{i=1}^4 z_i^2=\sum_{i=1}^4 y_i^2$. The determinant of the transformation is given by $|\partial y_i/\partial z_j|=(\gamma/4)^4$; moreover

$$z_1-z_2=(2/\gamma)^{1/2}(y_1+y_2) \qquad z_1-z_3=(2/\gamma)^{1/2}(y_1+y_3)$$
$$z_1-z_4=(2/\gamma)^{1/2}(y_2+y_3) \qquad z_2-z_3=(2/\gamma)^{1/2}(y_3-y_2) \tag{34}$$
$$z_2-z_4=(2/\gamma)^{1/2}(y_3-y_1) \qquad z_3-z_4=(2/\gamma)^{1/2}(y_2-y_1).$$

Thus from (3) the free energy is given by

$$\bar{f}_\gamma=\gamma(\ln 4-\tfrac{9}{8})+1$$
$$-\frac{1}{4}\ln\left(\frac{\int_0^\infty \Pi_{i=1}^3\,\mathrm{d}y_i^2\,\exp(-\Sigma_{i=1}^3 y_i^2)\int \Pi_{i=1}^3\,\mathrm{d}\varphi_i\,\Pi_{i<j}^3|y_i^4+y_j^4-2y_i^2y_j\cos(\varphi_i-\varphi_j)|}{(2\pi)^3 4!\,(\gamma/2)^4(\gamma/2)^{3\gamma}}\right)^{\gamma/2}. \tag{35}$$

We now carry out explicitly the computation for $\gamma=4$. Integration over the angles gives

$$\bar{f}_{\gamma=4}=4(\ln 4-\tfrac{9}{8})+1-\tfrac{1}{4}\ln\int_0^\infty \prod_{i=1}^3 \mathrm{d}y_i^2\,\exp\Big(-\sum_{i=1}^3 y_i^2\Big)\frac{1}{4!\,2^{16}}$$
$$\times(36a^2b^2c^2+4ac^2b^3+4a^3b^3+4abc^4+a^2b^4+\text{perm}).$$

where $a=y_1^4$, $b=y_2^4$, $c=y_3^4$ and perm means a permutation of a, b, c. We then obtain

$$\bar{f}_{\gamma=4}=8\ln 2-\tfrac{9}{8}+1-\tfrac{1}{4}\ln[(24)^3 1106(4!\,2^{16})^{-1}]=1.476\,613\,0$$

and $\bar{\bar{f}}_{\gamma=4}=1.068\,393\,8$. In the same way, using the binomial formula in (35), integrating over the angles and the moduli we obtain the free energy for $N=4$ up to $\gamma=14$ and the results are given in table 4.

Table 4.

γ	$\bar{f}_\gamma$	$\bar{\bar{f}}_\gamma$
2	0.493 142 9	0.901 362 0
4	1.068 393 8	1.476 612 9
6	1.442 088 1	1.850 307 1
8	1.726 747 9	2.134 967 0
10	1.958 902 1	2.367 121 2
12	2.155 684 8	2.563 903 9
14	2.326 839	2.735 058 8

Using (28) with $c=0$ as well as the results of tables 4 and 1 we obtain our extrapolated results as given in table 5.

Table 5.

γ	$\bar{\bar{f}}_\gamma(0)$	$\bar{f}_\gamma(0)$	equation (29)
2	0.822 51	0.831 99	0.826 27
4	1.262 93	1.272 54	1.255 03
6	1.574 24	1.583 884	1.579 062
8	1.840 13	1.849 765	1.849 042 4
10	2.080 75	2.090 388	2.085 569
12	2.298 225	2.307 86	2.299 237 2
14	2.419 432	2.501 09	2.496 260 2

The above estimates obtain with $N=2, 3, 4$ are much better than the ones obtained before with $N=1, 2, 3$. In fact, the method of extrapolation with $c=0$ in (28) fails to work for $\gamma>10$ and $N=1, 2, 3$, due to the fact that $x=1/N$ is not small enough at $N=1$; this is not the case for the extrapolation with $N=2, 3, 4$ particles and the computation confirms that the method yields fast convergent asymptotic limits for the free energy.

At a heuristic level, it is also of interest to consider an ansatz given by (29) which may give an approximate description of the thermodynamics of the system for not too large values of γ. We determine the parameters in (29) in requiring that (29) give the exact values for the free energy $f_\gamma=(\bar{f}_\gamma+\bar{\bar{f}}_\gamma)/2\gamma$ at $\gamma=14$, $\gamma=10$ and $\gamma=6$. We then found $c=4.315\,615$, $b=0.186\,781\,3$ and $a=0.044\,888$ in (29). The ansatz (see table 5) turns out to give an accurate description of the extrapolated results obtained with $N=2, 3, 4$ up to $\gamma=14$ which agrees reasonably with that of a Monte Carlo simulation of the system with $N=36$ in which a, b, c are slightly different, i.e. $a=0.017$, $b=0.225$ and $c=3.75$. Our results are preliminary, and are presented in figure 1, together with those of a Monte Carlo simulation of the system (Calinon and Choquard 1979, see also Choquard *et al* 1980b); a systematic computer computation of multiple integrals is in progress for N up to 6 and we believe that the approach will yield very accurate results for the free energy and correlation energy up to $\gamma=200$.

5. The virial pressure

For the model defined on a circular domain the one-body correlation function is rotationally invariant and it can be easily shown that the virial pressure is equal to the normalised density at the wall (Choquard *et al* 1980a, Calinon and Merlini 1982). Thus

$$\beta p_v/\rho = f_1(R) \tag{36}$$

where $f_1(x)$ is the one-body correlation function given by (7). At the present time we have not found any method of extrapolation for p_v analogous to that given by (28) for the free energy; this appears difficult since even at $\gamma=2$ the explicit N-dependence in (11) is very complicated. To obtain an estimate for p_v in the thermodynamic limit we use here a linear extrapolation of the exact results for $N=1$ and $N=2$, by means of the small polynomials given in § 2 for γ in the range $2 \leqslant \gamma \leqslant 14$. As remarked in § 2, the upper limit of integration in (11) cannot be taken equal to infinity as for the free energy, otherwise one would obtain the thermal pressure as we have shown explicitly for $\gamma = 2$ (equation (13)).

Let us first consider the case $\gamma = 2$, i.e.

$$\left(\frac{\beta p_v}{\rho}\right)_{\gamma=2} = \sum_{K=0}^{N-1} \frac{e^{-N} N^K}{\int_0^N \exp(-z^2) z^{2K} \, dz^2}.$$

The computation up to $N = 10$ is easily done and the results are given in table 6. With $x = 1/N$, let $\bar{p}_n$ be the value determined by (p_n, p_{n+1}) at $x = 0$, $n = 1, 2, \ldots, 10$ (linear extrapolation). We then obtain the sequence $\bar{p}_6 = 0.672\,164$, $\bar{p}_7 = 0.673\,658$, $\bar{p}_8 = 0.674\,869$, $\bar{p}_9 = 0.675\,879$. Defining in the same way $\bar{\bar{p}}n = (\overline{\bar{p}_n})$, we obtain $\bar{\bar{p}}_5 = 0.681\,709$, $\bar{\bar{p}}_6 = 0.682\,622$, $\bar{\bar{p}}_7 = 0.683\,346$, $\bar{\bar{p}}_8 = 0.684$. The last value may be compared with the exact value (Choquard 1980)

$$\lim_{N\to\infty} (\beta p_v/\rho)_{\gamma=2}(N) = \ln 2 = 0.693\,15$$

in the thermodynamic limit, and the error is 9×10^{-3}.

Table 6. Wall density at $\gamma = 2$ for $N = 1, 2, \ldots, 10$.

N	$p_N = \beta p_v(N)/\rho$
1	0.581 976 6
2	0.612 196 4
3	0.627 313 9
4	0.636 469 9
5	0.642 713 3
6	0.647 303 6
7	0.650 855 1
8	0.653 705 5
9	0.656 057 0
10	0.658 039 2

For $\gamma \geqslant 2$ a linear extrapolation of the results for $N = 1$ and $N = 2$ up to $\gamma = 12$ yields an estimate of $(\beta p_v/\rho)_\gamma$ in the thermodynamic limit as given below. The values of table 7, equation (12) and the results of a Monte Carlo simulation with $N = 37$ particles are plotted in figure 2. As can be seen the agreement is satisfactory. To

Table 7. The viral pressure up to $\gamma = 12$.

γ	$(\beta p_v/\rho)$	Monte Carlo
0	1	1
2	0.642 492 8	0.647 2
4	0.426 622 4	0.423 5
6	0.282 297 6	0.269 9
8	0.182 545 2	0.168 1
10	0.079 635 8	0.077 8
12	0.070 120 4	—

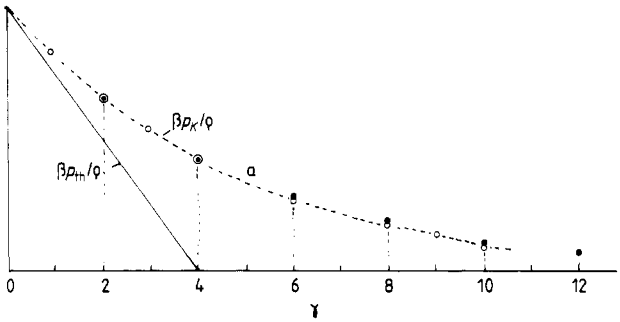

Figure 2. The kinetic pressure from a Monte Carlo computation with $N=37$ particles (Calinon and Choquard 1979, see also Choquard *et al* 1980b), curve a with open circles; the full circles are our results of table 7, and the thermal pressure (12).

conclude this section, it should be remarked that, as for the computation of the free energy density, the thermodynamic limit may not be said to be completely reached, so that a possible non-analytic behaviour at large values of γ may not be discovered within a Monte Carlo simulation with $N=37$ or within the present treatment with $N=1$ and $N=2$. The results of both treatments indicate that the pressure is a positive monotonically decreasing function of γ up to $\gamma=12$.

6. Conclusions

In this work we have presented an analytical approach and a method of extrapolation to compute the thermodynamics of the two-dimensional one-component plasma. Preliminary results up to moderately high values of the coupling parameter $\gamma \sim 14$ have been obtained for the free energy and the kinetic pressure of the system. They agree reasonably well with that of the first Monte Carlo computer experiment on the system which was carried out with $N=37$ particles (Calinon and Choquard 1979, see also Choquard *et al* 1980b). In addition recently new refined and Monte Carlo computer experiments with more particles (Caillol *et al* 1982), as well as molecular dynamics computations (De Leeuw and Perram 1982), indicate that the two-dimensional system (as in three dimensions) has the interesting property of undergoing a first-order phase transition at high values of the plasma parameter γ situated in the range $\gamma \sim 135$–140. The question if the transition which takes place in the system is connected with a symmetry breakdown of the translation group (appearance of periodic states with long-range positional order), or if it concerns the appearance of long-range directional order only, is still open. In connection with the above situation, it is interesting to note that the free energy is independent of boundary condition (Albeverio *et al* 1982). It thus follows that to investigate a possible non-analytic behaviour of the free energy as a function of γ, it is sufficient to consider the model on a circular domain with open boundary condition as has been considered in this work. Moreover, it has been shown that long-range positional order (appearance of a crystalline phase) with periodic electron density in the thermodynamic limit cannot occur in the system, except possibly if the pair correlation function $g(\boldsymbol{r})$ decays more slowly than $1/r^2$ for $r\to\infty$ (Martinelli and Merlini 1982); at the present time a study of the behaviour of $g(r)$ to show a slower decay then $1/r^2$ at high values of γ has not been considered in the Monte Carlo or molecular-dynamic treatments and this appears difficult; we expect that further computations along the lines developed in this note should give an accurate description of the thermodynamic free energy and internal energy exact up to 10^{-5}, so that a possible non-analytic behaviour could be detected, as a manifestation of a phase transition (Johannesen and Merlini 1982).

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References

Alastuey A and Jancovici B 1981 *J. Physique* **42** 1–10
Albeverio S, Dürr D and Merlini D 1982 *J. Stat. Phys.* **30** to appear
Bakshi P, Calinon R, Golden K, Kalman G and Merlini D 1979 *Phys. Rev.* A **20** 339–41
—— 1981 *Phys. Rev.* A **23** 1925–36
Caillol J M, Levesque D, Weiss J J and Hansen J P 1983 *J. Stat. Phys.* **30** to appear
Calinon R and Choquard Ph 1979 presented at *Int. Conf. Mathematical Physics, Lausanne, Switzerland*
Calinon R, Golden K, Kalman G and Merlini D 1979 *Phys. Rev.* A **20** 327–39
Calinon R and Merlini D 1982 *Preprint, Phys. Fluids* to appear 1983
—— 1982 *Lett. Nuovo Cimento* **33** 485–90
Choquard Ph 1978 *Helv. Phys. Acta* **51** 435–6
—— 1980 (private communication)
Choquard Ph, Favre P and Gruber C 1980a *J. Stat. Phys.* **23** 405–27
Choquard Ph, Jamin D and Navet J 1980b in *Ordering in Two-dimension, Proc. Int. Conf. Lake Geneva, Wisconsin, May 1980* ed S K Sinha (New York: North-Holland)
De Leeuw S W and Perram J W 1982 *Preprint*
Deutsch C, Dewitt H E and Furutani Y 1979 *Phys. Rev.* A **20** 263–8
Gann R C, Chakravartz S and Chester G V 1979 *Phys. Rev.* B **20** 325–33
Golden K and Merlini D 1977 *Phys. Rev.* A **16** 438–42
Hauge E H and Hemmer P C 1971 *Phys. Norv.* **5** 209–20
Jancovici B 1981a *Phys. Rev. Lett.* **46** 386–90
—— 1981b *J. Physique Lett.* **42** 223–8
Johannesen S and Merlini D 1982 *Phys. Lett.* **93**A 21–4 (and work in preparation)
Malmberg J H and O'Neil T M 1977 *Phys. Rev. Lett.* **39** 1334–6
Martinelli F and Merlini D 1982 '*Refined Mermin's argument for the two-dimensional jellium*' submitted to *J. Stat. Phys.*
Mehta M L 1967 *Random Matrices* (New York: Academic)
Prasad S A and O'Neil T M 1979 *Phys. Fluids* **22** 279–81
Sari R, Calinon R and Merlini D 1976 *J. Phys. A: Math. Gen.* **9** 1539–51
Sari R and Merlini D 1976 *J. Stat. Phys.* **14** 91–100
Schwarz L 1965 *Méthodes Mathématiques pour les Sciences Physiques* (Paris: Hermann)