CLM-P350

E·MINIMIS·MAXIMA

UKAEA RESEARCH GROUP

Preprint

NEGATIVE TEMPERATURE STATES OF TWO DIMENSIONAL PLASMAS AND VORTEX FLUIDS

S F EDWARDS
J B TAYLOR

CULHAM LABORATORY
Abingdon Berkshire

1973

CLM-P 350

NEGATIVE TEMPERATURE STATES OF TWO DIMENSIONAL PLASMAS AND VORTEX FLUIDS

by

S.F. EDWARDS[†], F.R.S. and J.B. TAYLOR, F.R.S.

(Submitted for publication in Proc. Roy. Soc. A)

ABSTRACT

The two dimensional guiding centre plasma and a system of interacting line vortices in an ideal fluid are examples of Hamiltonian systems with bounded phase space. The statistical mechanics of such systems is investigated. An interesting feature is that they can exist in negative temperature states which show observable intrinsic characteristics, such as the formation of clusters of particles.

---

† Permanent address: Cavendish Laboratory, University of Cambridge

UKAEA Research Group,
Culham Laboratory,
Abingdon,
Berks.

July 1973

INTRODUCTION

There has recently been considerable interest (Taylor & McNamara 1971; Vahala & Montgomery 1971; Dawson, Okuda & Carlile 1971; Montgomery 1972 a,b,c; Taylor 1972 a,b; Montgomery & Tappert 1972; Taylor & Thompson 1973; Okuda & Dawson 1973; Christiansen & Taylor 1973; Lee & Lin 1973) in the two dimensional guiding centre model of a plasma. This model is one in which long filaments of charge are aligned parallel to a uniform magnetic field $\underset{\sim}{B}$ and move under their mutual electric field $\underset{\sim}{E}$ with the 'guiding centre' velocity $(\underset{\sim}{E} \times \underset{\sim}{B})/B^2$. The equations of motion are

$$e_i \frac{dx_i}{dt} = \frac{1}{B}\frac{\partial H}{\partial y_i} \qquad e_i \frac{dy_i}{dt} = -\frac{1}{B}\frac{\partial H}{\partial x_i} \tag{1}$$

where e_i/ℓ is the charge per unit length of the filament and H is the coulomb interaction energy

$$H = \sum_{i<j} -\frac{2e_i e_j}{\ell} \log \left|\underset{\sim}{r}_i - \underset{\sim}{r}_j\right| . \tag{2}$$

A scale transformation makes these equations identical with those for the motion of interacting parallel line vortices in an incompressible non-viscous fluid (Onsager 1949; Lin 1943); the charge e_i is replaced by the strength (circulation) of the i^{th} vortex.

The two dimensional plasma and the vortex fluid are thus described by the same dynamical equations. An interesting feature of this dynamics is that the force acting on a "particle" determines its velocity rather than its acceleration. This may be regarded as being brought about by the absence of any kinetic energy term in the Hamiltonian. Moreover, since x_i, y_i are essentially the conjugate coordinates these systems also have the property that their phase space is bounded - it cannot exceed V^{2N}, where V is the volume (area) of the system and 2N the number of particles. From the viewpoint of statistical mechanics this limitation is the most important property and we shall refer to systems such as the plasma or vortex models as limited phase space systems.

In this paper the equilibrium statistical mechanics of these systems is investigated; in addition to its possible interest for real plasmas or fluids this is of interest for the interpretation of recent computer simulations of plasmas and fluids (Montgomery 1972 b; Dawson et.al. 1971; Joyce & Montgomery 1973; Christiansen & Taylor 1973). It will turn out that, because of the long range of the coulomb force, the interaction (2) does not lead to conventional thermodynamic limits as the volume increases. The micro-canonical and canonical ensembles are therefore not equivalent for systems with the interaction potential (2) and concepts such as temperature and pressure require careful consideration. In order to bring out these points we shall also consider a modified form of interaction potential in which the long range effects are absent and for which conventional thermodynamic limits do exist.

The first application of statistical arguments to the vortex fluid system was by Onsager (1949). He noted that because of the limitation on the total phase space, negative "temperatures" would occur when the energy of the system exceeded some critical value. Recently Taylor (1972a) determined the approximate value of this critical energy. Further investigations have since been made by Joyce and Montgomery (1973), in conjunction with numerical simulations, who observed that a form of condensation may occur in the negative temperature regime.

A second unusual feature of systems with the coulomb interaction (2) was first noted by Salzberg and Prager (1963). They observed that for such systems one may derive an exact equation of state which formally predicts negative pressures below some critical temperature T_c.

In our investigation of these phenomena we shall take as our model a system of N positive particles (or vortices) of strength $e_i = e$ and an equal number of negative particles of strength $e_i = -e$ in a finite two dimensional 'volume' V. The mean density of either species is thus $n = N/V$. We shall put $\ell = 1$ for convenience so that $e^2/\ell = e^2$ is to be regarded as an energy.

THE CHOICE OF ENSEMBLE

In the standard manner, the equilibrium properties of our system are assumed to be given by regarding it as a member of an ensemble with an appropriate distribution. If the temperature were specified, by contact with a heat bath, the appropriate distribution would be the Gibbs canonical distribution $\exp(-H(x_i, y_i)/kT)$. However the concept of a heat-bath is not appropriate in the present context as we do not have readily available negative temperature heat baths, either in reality or in computer simulations. Instead we shall consider a completely isolated system for which the appropriate distribution is the micro-canonical distribution

$$\rho(x_i,y_i) \sim \delta(E - H(x_i,y_i)).$$

In the microcanonical distribution the energy is specified exactly; in the canonical distribution the energy fluctuates about the mean value. For normal systems these fluctuations are negligible when the number of particles is large and the two ensembles are equivalent but as we have already indicated this is not the case for systems with the coulomb potential (2).

With the microcanonical ensemble it is convenient to introduce two structure functions; $\phi(E)$ the volume of phase space whose energy is less than E, and the statistical weight

$$\Omega(E,V,N) = \frac{d\varphi}{dE} = \int \delta(E - H(x_i,y_i))d\Omega \ .$$

Then the entropy is

$$S(E,V,N) = \log \Omega(E,V,N)$$

and all other thermodynamic quantities may be derived from this. When the thermodynamic limit exists the temperature T and the pressure P have their conventional significance and are given by

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{V,N} \qquad (3)$$

and

$$P = -\left(\frac{\partial E}{\partial V}\right)_{S,N} = \left(\frac{\partial S}{\partial V}\right) \cdot \left(\frac{\partial S}{\partial E}\right)^{-1} \qquad (4)$$

when no such limit exists these equations will be taken to define temperature and pressure.

EQUATION OF STATE

An exact equation of state can be derived for a two dimensional system with coulomb forces. We first introduce an explicit representation of the δ-function so that

$$\Omega = \int \frac{d\lambda}{2\pi} \ \exp\left(i\lambda\left(E + \sum{}' e_i e_j \log r_{ij}\right)\right) \Pi \ d\underset{\sim}{r}_i \qquad (5)$$

where Σ' denotes that terms $i = j$ are excluded from the summation. Then, following Salzberg and Prager (1963), we make a scale transformation $r \to r' V^{\frac{1}{2}}$ so that

$$\Omega = \frac{V^{2N}}{2\pi} \int d\lambda \, \exp\left(i\lambda \left(E + \sum{}' \frac{e_i e_j}{2} \log V + \sum{}' e_i e_j \log r'_{ij} \right)\right) \Pi \, d\underset{\sim}{r}'_i$$

where the r'_i integrations are now independent of the volume V. Since there is an equal number of positive and negative particles $\Sigma' e_i e_j = -Ne^2$ and

$$\Omega = \frac{V^{2N}}{2\pi} \int d\lambda \, \exp\left(i\lambda E - \frac{i\lambda Ne^2}{2} \log V \right) \int \exp\left(i\lambda \sum{}' e_i e_j \log r'_{ij} \right) \Pi \, dr' \quad .$$

Direct differentiation now formally yields the equation of state

$$PV = 2NT(1 - e^2/2T) \tag{6}$$

where P,T are defined by (3) and (4). This is identical with the equation derived by Salzberg and Prager from the conventional partition function.

A striking feature of (6) is that the pressure becomes <u>negative</u> for temperatures less than $T_c \equiv e^2/2$. However further investigation shows that the regime below $2T_c$ is unattainable. This is a consequence of the behaviour of (5) for small r_{ij} and reflects a physical condensation of the system into neutral pairs (Hauge & Hemmer 1971); it does not affect the rest of our investigation which is concerned with long range phenomena.

We shall, however, discuss in detail another negative pressure regime, namely that in which <u>the temperature is also negative.</u> This regime <u>is</u> attainable. There is again a form of condensation but in this case it is long range, involving many particles rather than pairs. As mentioned earlier , the existence of this negative temperature regime was noted by Onsager (1949) whose argument runs as follows. The total phase space is bounded and $\emptyset(E) \to V^{2N}$ as $E \to +\infty$; consequently $\emptyset'(E)$ must have a maximum at some finite value E_m of E. The temperature

$$T = \emptyset''(E)/\emptyset'(E)$$

must therefore be negative when $E > E_m$.

ENTROPY

The exact equation of state gives no information on the relation between entropy and energy. This can be found only by introducing approximate methods, based on the fact that the number of particles is large.

We first introduce the fourier transforms $p_{\underset{\sim}{k}}$, $q_{\underset{\sim}{k}}$ of the density of positive and negative charges respectively

$$p_{\underset{\sim}{k}} = \frac{e}{V} \sum_{+} \exp(i\,\underset{\sim}{k}.\underset{\sim}{r}_i) \qquad q_{\underset{\sim}{k}} = \frac{e}{V} \sum_{-} \exp(i\,\underset{\sim}{k}.\underset{\sim}{r}_j) \tag{7}$$

where the allowed values of k are such that $k_x.L = 2\pi$ (integer) etc. We define

$$\rho_k = (p_k - q_k) \text{ and } \eta_k = (p_k + q_k) \ ,$$

then the interaction energy is

$$H = 2\pi V \sum_k (|\rho_k|^2 - \frac{4\pi N e^2}{V^2}) \cdot \frac{1}{k^2} \ . \tag{8}$$

The essential step (Edwards 1958; Taylor & McNamara 1971) is to employ a set of the $\{\rho_k, \eta_k\}$ as variables of integration in place of the $\{\underset{\sim}{r}_i, \underset{\sim}{r}_j\}$. For large N the Jacobian of the transformation is

$$J = V^{2N} \prod \frac{V^2}{2Ne^2} \exp\left(- \frac{V^2}{2Ne^2} (|\rho_k|^2 + |\eta_k|^2) \right) \ . \tag{9}$$

[This expression may be verified by recalling that the Jacobian can be interpreted as the density in (ρ_k, η_k) space when there is a uniform density in $\{\underset{\sim}{r}_i, \underset{\sim}{r}_j\}$ space. This (ρ_k, η_k) distribution can be found from the moments of ρ_k and η_k of which the only non-zero ones are

$$< |\rho_k^{2m}| > = < |\eta_k^{2m}| > = m! \quad (Ne^2/V^2)^m$$

when N is large. Alternatively, again interpreting it as the distribution of (ρ_k, η_k) when the $\{\underset{\sim}{r}_i, \underset{\sim}{r}_j\}$ are uncorrelated, one may regard (9) as an application of the central-limit theorem.]

As the Jacobian and the energy involve only $|\rho_k|$ we set $\rho_k = r_k \exp i\,\phi_k$. The integrations over ϕ_k and over η_k play no significant role in the calculation and the statistical weight (5) becomes;

$$\Omega = \frac{V^{2N}}{2\pi} \int d\lambda \prod_k dr_k^2 \left\{ \frac{V^2}{2Ne^2} \exp\left(\frac{-V^2}{2Ne^2} \cdot r_k^2 \right) \right\} \exp i\lambda E$$

$$\cdot \exp\left\{ 2\pi i\lambda V \sum_k (r_k^2 - \frac{4\pi N e^2}{V^2}) \cdot \frac{1}{k^2} \right\} . \tag{10}$$

The integrations over r_k then give

$$\Omega = \frac{V^{2N}}{2\pi} \int d\lambda \; \exp \; i\lambda E \quad \underset{k}{} \left\{ \frac{\exp(i\alpha^2\lambda/k^2)}{(1 + i\alpha^2\lambda/k^2)} \right\} \tag{11}$$

where $\alpha^2 \equiv 4\pi m e^2$. The integrand is singular whenever $\lambda = ik^2/\alpha^2$. Equation (11) may also be written in the more convenient form

$$\Omega = \frac{V^{2N}}{2\pi} \int d\lambda \; \exp \left\{ i\lambda E - \sum_k \left(\log \left(1 + \frac{i\alpha^2\lambda}{k^2} \right) - \frac{i\alpha^2\lambda}{k^2} \right) \right\} . \tag{12}$$

At this point one would like to take the limit $N \to \infty$, $V \to \infty$, N/V constant, treating S and E as extensive variables (proportional to volume) as in thermodynamics. This would lead to a thermodynamic relation of the type

$$\frac{S}{N} = f \left(\frac{E}{N} , \frac{V}{N} \right),$$

and make the temperature

$$T = \left(\frac{\partial S}{\partial E} \right)^{-1} = h \left(\frac{E}{N} , \frac{V}{N} \right)$$

and intensive variable. However, due to the long range nature of the coulomb force no such thermodynamic limit exists for models with coulomb forces. We will take up the coulomb model again later but in order to remain within the framework of conventional thermodynamics we shall first introduce a modification of the model.

THE FINITE RANGE MODEL

The modification is merely to replace the long range coulomb potential by a finite range one. Specifically we replace the coulomb potential $1/k^2$ by the potential $1/(k^2 + a^2)$. In coordinate space this replaces $\log r_{ij}$ by $K_o(a\, r_{ij})$, with K_o a Bessel function of imaginary argument. The parameter a^{-1} is the characteristic range of the potential. It is important to realise that the introduction of this modified force does not alter the special properties of our system associated with limited phase volume.

With the modified form of interaction the statistical weight is

$$\Omega = \frac{V^{2N}}{2\pi} \int d\lambda \; \exp \left\{ i\lambda E - \sum \left(\log \left(1 + \frac{i\,\alpha^2\,\lambda}{(k^2 + a^2)} \right) - \frac{i\,\alpha^2\,\lambda}{(k^2 + a^2)} \right) \right\}. \tag{13}$$

In the limit $V \to \infty$ the summation over $\underset{\sim}{k}$ may be replaced by an integral

$$\sum_k \rightarrow \frac{V}{(2\pi)^2} \int d\underset{\sim}{k} = \frac{V}{2\pi} \int k dk ,$$

and performing this integration,

$$\Omega = \frac{V^{2N}}{2\pi} \frac{a^2}{4\pi e^2} \int \exp \frac{Va^2}{4\pi} \left\{ iz\epsilon + (1 + iz) \log (1 + iz) - iz \right\} dz \tag{14}$$

where $\epsilon = E/Ne^2$, and $z = 4\pi e^2\lambda/a^2$.

As $V \rightarrow \infty$ the integration over z can be carried out by the steepest descent method. The saddle point is at $iz = (\exp(-\epsilon)-1)$ and the final result of the integration is

$$S(E,V,N) = \frac{Va^2}{4\pi} \left[1 - \frac{E}{Ne^2} - \exp\left(\frac{-E}{Ne^2}\right) \right] + 2N \log V, \tag{15}$$

which is indeed of the thermodynamic form. Corrections to (15) are of order $1/a^2V$ so that the steepest descent evaluation is accurate in the limit $V \rightarrow \infty$. All thermodynamic quantities may be obtained from this expression.

The equation of state corresponding to eq.(15) is

$$\left[P - \frac{a^2T}{4\pi} \log\left(1 + \frac{4\pi e^2}{a^2T}\right)\right] V = 2N \left[T - \frac{e^2}{2} \right] \tag{16}$$

which differs from equation (6) for a coulomb system because of the introduction of the finite range force. This difference can be regarded as a change in the pressure by an amount which $\rightarrow 0$ as $a^2 \rightarrow 0$.

The temperature is given in terms of the energy of the system by

$$\frac{1}{T} = \frac{a^2}{4\pi e^2} \left[\exp\left(\frac{-E}{Ne^2}\right) - 1 \right] , \tag{17}$$

which is one of our most interesting results. It shows that the <u>temperature is negative</u> whenever the energy is positive, i.e., the critical energy E_m for the onset of negative temperatures is exactly $E_m = 0$. For large values of the energy, the temperature tends to a limiting negative value $- a^2/4\pi e^2$ and the accessible range of negative temperatures is therefore $- \infty < T < - a^2/4\pi e^2$.

<u>Negative Temperature Phenomena in the Finite Range Model</u>

Many of the unusual properties of negative temperature systems arise when they interact with other, positive temperature, systems. In such interaction heat flows <u>from</u> the negative temperature component to the positive temperature one. In this way the entropy of both systems is increased. However, one reason for interest in the present model is that some features associated with negative temperature are observable within the isolated system itself. To illustrate these we examine the spectrum of charge density fluctuations.

The spectrum of charge fluctuations is given (c.f. equation 10) by

$$< |\rho_\ell{}^2| > = \frac{V^{2N}}{\Omega} \int \frac{d\lambda}{2\pi} \; r_\ell^2 \prod dr_k{}^2 \left\{ \frac{V^2}{2Ne^2} \exp\left(\frac{-V^2}{2Ne^2}\, r_k^2\right) \right\} \exp\, i\lambda E$$

$$. \exp\left\{ -\, 2\pi\, i\, \lambda\, V \sum (r_k^2 - \frac{4\pi N e^2}{V^2}) \,.\, \frac{1}{(k^2 + a^2)} \right\} \qquad (18)$$

and after integrating over $r_k{}^2$,

$$< |\rho_\ell{}^2| > = \frac{2Ne^2}{V^2} \,.\, \frac{V^{2N}}{\Omega} \int \frac{d\lambda}{2\pi} \left(1 + \frac{i\alpha^2\lambda}{\ell^2 + a^2}\right)^{-1}$$

$$. \exp\left\{ i\lambda E - \sum \left(\log\left(1 + \frac{i\alpha^2\lambda}{(k^2 + a^2)}\right) - \frac{i\alpha^2\lambda}{(k^2 + a^2)}\right) \right\} . \qquad (19)$$

In the limit of large V we again replace the summation over k by integration and evaluate the integral over λ by the method of steepest descents. Then

$$< |\rho_\ell{}^2| > = \frac{2Ne^2}{V^2} \left[\frac{\ell^2 + a^2}{\ell^2 + a^2 \exp(-\epsilon)} \right] \qquad (20a)$$

or, in terms of the temperature,

$$< \rho_\ell{}^2 > = \frac{2Ne^2}{V^2} \left[1 + \frac{4\pi m e^2}{(\ell^2 + a^2)T} \right]^{-1} \,. \qquad (20b)$$

Equation (20) shows that when $\epsilon = 0$ ($T = \infty$) the spectrum is flat, as for a random distribution of charges (Taylor & Thompson 1973). When $\epsilon < 0$ (positive temperature) the spectrum is depressed at small k, i.e. long wave fluctuations are reduced. This is similar to the Debye shielding effect in normal coulomb plasmas. On the other hand when $\epsilon > 0$ (negative temperature) the spectrum is enhanced at small k and long wave fluctuations are increased.

This enhancement of long wavelength fluctuations in the negative temperature regime corresponds to a form of "anti-shielding" in which each particle is surrounded by a cloud of similar particles. A picture of this cloud is provided by the charge correlation function

$$< \rho(\underset{\sim}{r})\ \rho\ (\underset{\sim}{r} + \underset{\sim}{s}) > = \Sigma < |\rho_k^2| > \exp\ (i\,\underset{\sim}{k}\,.\,\underset{\sim}{s})$$

which can be written

$$< \rho(\underset{\sim}{r})\ \rho\ (\underset{\sim}{r} + \underset{\sim}{s}) > \ = \frac{2Ne^2}{V} \left\{ \delta(\underset{\sim}{s}) + \frac{a^2}{2\pi}\ (1 - \exp\ (-\ \epsilon))K_o(s\ a \exp\ (-\ \epsilon/2)) \right\} . \tag{21}$$

The second term in this correlation function arises from the charge cloud which, on average, accompanies each particle. The radius of the cloud is $\sim a^{-1}$ exp $(\epsilon/2)$. If $\epsilon < 0$ the cloud is of opposite sign to the particle and shields its effect. However if $\epsilon > 0$ the cloud is of the same sign as the particle and enhances its effect. By integrating (21) we can obtain the total effective charge in the shielding or reinforcing cloud; this is

$$q_s = (\exp(\epsilon) - 1)e. \tag{22}$$

In the negative temperature regime ($\epsilon > 0$) the charge fluctuations in the system can be regarded as due to the formation of large 'clumps' or 'clusters' of charge, each cluster containing $\sim$ (exp(ϵ) - 1) particles and growing in size as the energy increases.

For a limited phase system with short range forces, then, there is a proper thermodynamic entropy (15) and a temperature which is negative whenever the energy exceeds zero. This negative temperature regime is characterised by a greatly enhanced level of macroscopic fluctuations and a tendency for <u>like</u> particles to form clumps or clusters. We now return to the coulomb model to investigate to what extent similar phenomena occur in that model despite the absence of a proper thermodynamic limit.

THE COULOMB SYSTEM

For the coulomb case the statistical weight (12), writing $k^2 = (4\pi^2/V)\kappa^2$ where κ is independent of volume, becomes

$$\Omega = \frac{V^{2N}}{Ne^2} \int \frac{dz}{2\pi} \prod \left(1 + \frac{iz}{\pi\kappa^2}\right)^{-1} \exp \left(iz\epsilon + iz\ \Sigma \frac{1}{\pi\kappa^2}\right) . \tag{23a}$$

The entropy thus has the form

$$S = 2\ N \log V - \log Ne^2 + \log\ (g(E/N))$$

and so does not tend to an extensive limit as $E,V,N \rightarrow \infty$ with E/N and V/N finite. Consequently the temperature defined by

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right) = \frac{1}{N}\ g'\ (E/N)$$

is not an intensive quantity in this limit. Indeed the temperature will depend on the shape of the container!

To investigate (23a), it is useful to write it as

$$\Omega = \frac{V^{2N}}{Ne} \int \frac{dz}{2\pi} \exp\left\{ iz\epsilon - \sum_{\kappa} \left(\log\left(1 + \frac{iz}{\pi\kappa^2}\right) - \frac{iz}{\pi\kappa^2} \right) \right\} \qquad (23b)$$

and to replace the sum over κ by an integral, (but the error in this approximation is no longer asymptotically small as $V \to \infty$; indeed the error is independent of V). Then

$$\Omega = \frac{V^{2N}}{Ne^2} \int \frac{dz}{2\pi} \exp\left\{ iz\epsilon + \pi b^2 \left[\left(1 + \frac{iz}{\pi b^2}\right) \log\left(1 + \frac{iz}{\pi b^2}\right) - \frac{iz}{\pi b^2} \right] \right\} \qquad (24)$$

where b is the lower cut-off in the κ integration. It is appropriate and convenient to take $\pi b^2 = 1$, when the entropy becomes

$$S = \log \Omega = 2N \log V + \log(g(\epsilon)), \qquad (25)$$

where

$$g(\epsilon) \equiv \int \frac{dz}{2\pi} \exp\left(iz\epsilon + (1 + iz)\log(1 + iz) - iz\right) \cdot \qquad (26)$$

The exponent in this integral, like that in (14), has a saddle point at $(1 + iz) = \exp(-\epsilon)$ but the steepest descent method is no longer automatically validated by a large parameter V. Nevertheless on deforming the contour appropriately one finds that the steepest descent approximation to equation (26) is accurate when ϵ is large and negative. In this regime

$$\log(g) \simeq 1 - \frac{3}{2}\epsilon - \exp(-\epsilon) \qquad (27)$$

and the entropy is

$$S = 2N \log V - \frac{3E}{2Ne^2} - \exp\left(\frac{-E}{Ne^2}\right). \qquad (28)$$

The temperature $(\partial S/\partial E)^{-1}$ is therefore given by

$$\frac{1}{T} = \frac{1}{Ne^2} \left[\exp\left(\frac{-E}{Ne^2}\right) - \frac{3}{2} \right] \qquad (29)$$

which is negative when $E > E_m = -(\log 3/2)\, Ne^2 \simeq -0.405\, Ne^2$.

Another expression for $g(\epsilon)$ can be obtained by noting that the integrand in (26) has a branch point at $z = +i$. We therefore introduce a cut from i to $i\infty$ along the imaginary axis and the contour of integration may then be deformed to lie along the edges of the cut. Observing that arg z differs by 2π on the two edges of the cut, and writing $1 + iz = ix$,

$$g(\epsilon) = \angle \exp(1-\epsilon)\int_0^\infty (\operatorname{Sin} \pi x) \exp(x - x \log x - \epsilon x)dx. \tag{30}$$

This integral is convenient for numerical evaluation of g, and therefore of the entropy. Such numerical evaluation shows that the saddle point approximation (27) is accurate to better than 3 % when $\epsilon < 0$. In particular the value for the threshold of negative temperatures obtained numerically is $E_m = -0.393\ Ne^2$ which agrees remarkably well with that from the saddle point approximation.

When ϵ is positive the saddle point approximation is not valid. It is then more convenient to return to (23a) and consider the residue from each of the poles at $z = i\pi\kappa^2$ after closing the contour in the upper half plane. When $|\epsilon| \gg 1$ the dominant contribution is that from the pole nearest the real axis, whose contribution is of the form

$$\epsilon^{p-1} \exp(-\gamma\epsilon)$$

where p is the degeneracy of the mode of longest wavelength and γ is a number of order unity depending on the shape of the container. As $\epsilon \to \infty$, therefore, the entropy becomes

$$S \simeq -\frac{\gamma E}{Ne^2} + (p-1)\log\left(\frac{E}{Ne^2}\right), \tag{31}$$

and the temperature tends to

$$\frac{1}{T} = -\frac{\gamma}{Ne^2} .$$

The range of accessible negative temperatures for the coulomb system is therefore $-\infty < T < -\gamma/Ne^2$.

We see from these results that, despite the absence of the usual thermodynamic limit, the coulomb system has many features similar to those of the short range model. In particular when the energy exceeds the threshold $E_m \simeq -0.4\ Ne^2$ the entropy is a decreasing function of the energy, i.e. the "temperature" is negative. It is also interesting that the steepest descent method is valid for a coulomb system when $\epsilon \ll -1$. For in this case the micro-canonical and canonical ensembles must lead to similar results. According to (29) the requirement that $\epsilon \ll -1$ is equivalent to

$$\frac{Ne^2}{T} \gg + 1$$

which can be interpreted as a requirement that the Debye length $(T/ne^2)^{\frac{1}{2}}$ be much less than the dimensions of the system.

Negative Temperature Phenomena in the Coulomb System

As for the short range model we first calculate the fluctuation spectrum $< |\rho_k^2| >$ which is given by

$$< |\rho_k^2| > = \frac{2Ne^2}{V} \cdot \frac{1}{\Omega} \int \frac{k^2V}{(k^2V + 4\pi iz)} \prod \left\{ \left(1 + \frac{iz}{\pi K^2}\right)^{-1} \right\}$$

$$. \exp\left(i z \epsilon + i z \; \Sigma \; \frac{1}{\pi K^2} \right) dz \; . \qquad (32)$$

This expression can be evaluated by similar approximations to those used for Ω itself. In the regime $\epsilon \ll - 1$, (positive temperatures) the ste-epest descent method can be used and leads to

$$< |\rho_k^2| > = \left[1 + \frac{4\pi}{k^2V} \left(\exp(-\epsilon) - 1\right) \right]^{-1} = \left(1 + \frac{4\pi ne^2}{k^2T} \right)^{-1} \qquad (33)$$

which is the conventional value, showing suppression of long wave fluctuations by Debye shielding.

In the strongly negative temperature regime $\epsilon \gg 1$ the integral in equation (32) can be evaluated directly by residues, with the dominant contribution again coming from the pole nearest the real axis. For the longest wave length mode the order of the dominant pole in the integral (32) exceeds the order of the (same) dominant pole in Ω by unity and

$$< |\rho^2| > = \frac{2Ne^2}{V^2} \; \epsilon \; . \qquad (34a)$$

However for all other wavelengths the order of the dominant pole is the same in the integral and in Ω itself. Consequently for all modes other than the longest one,

$$< |\rho^2| > = \frac{2Ne^2}{V^2} \; . \qquad (34b)$$

In the coulomb system therefore, a <u>single</u> mode (or group of equivalent modes if the longest wavelength is degenerate) is enhanced above all others when the temperature is negative, the rest of the spectrum being flat as for random particles.

Although this enhancement of the longest mode again corresponds to a tendency for like particles to cluster together, the size of the clusters is not now an intrinsic property of the system but is fixed by the size and shape of the container. The clustering will simply produce a modulation in the charge density corresponding to the longest mode, or group of modes. The amplitude of this modulation is $\sim \epsilon^{\frac{1}{2}}(Ne^{\frac{1}{2}}/V) = (E^{\frac{1}{2}}/V)$ and so increases rather slowly with the energy of the system.

CONCLUSIONS

We have investigated the statistical mechanics of two dimensional limited phase space systems, of which the guiding centre plasma and the vortex fluid are the prototypes, with two forms of interaction between particles - the long range coulomb force and a short range force.

With the short-range-force an asymptotic limit exists as $V \to \infty$ and leads to an extensive entropy (15) from which all thermodynamic quantities can be obtained. The temperature, given by (17), exhibits the characteristic feature of limited phase space systems, namely that their temperature becomes <u>negative</u> when their energy is sufficiently large. In fact for the short range case this critical energy is $E_m = 0$.

These negative temperature states are of special interest in the present model because, in addition to thermodynamic properties shared by any negative temperature system, they exhibit observable internal characteristics attributable to the negative temperature. These are a high level of macroscopic fluctuations and the (related) tendency to form macroscopic clusters of similar particles. The size of each cluster and the number of particles in it both increase with the energy of the system in a manner which we have calculated.

With the coulomb potential we do not find the usual thermodynamic limit as the volume tends to infinity and the entropy is not an extensive function of the energy per particle. Nevertheless, in the limits $E/Ne^2 \ll -1$ and $\gg +1$ explicit expressions have been derived for the entropy. The "temperature" $(\partial S/\partial E)^{-1}$, although not an intensive variable, is again negative when the energy of the system exceeds a threshold value. This threshold is no longer exactly $E_m = 0$; we have estimated it to be $E_m \simeq -0.4\ Ne^2$.

The characteristics of the negative temperature state for the coulomb model are different to those of the short range model. There are enhanced fluctuations but the single longest wavelength mode (or group of degenerate modes) is preferentially excited. Consequently although clustering again occurs it is now controlled by the size and shape of the system. One expects only a single positive and a single negative cluster such as will produce a modulation in the charge density of amplitude $(E^{\frac{1}{2}}/V)$. This corresponds roughly to all the "surplus" energy above the threshold value E_m appearing in this macroscopic mode (Joyce & Montgomery 1973).

This clustering behaviour was first noted by Joyce & Montgomery and illustrated by them with numerical simulations of the coulomb system in a rectangular box. Similar numerical simulations carried out by J.P. Christiansen and one of us (J.B.T) are shown in figs. 1 - 4. In these simulations the motion of several thousand particles interacting through the coulomb force were followed by the VORTEX code (Christiansen 1970; Christiansen & Taylor 1973). The system is periodic in both directions and the electric field is calculated at each time step by a fast fourier transform method on a 64 × 64 mesh. Initially, positive and negative particles are distributed on alternate squares of a chequered pattern (fig.1) and the energy of the system is selected by changing the size (but not the number) of the squares. The particles are then followed for as long as limitations of computer time and accuracy will allow.

A typical final state of the system for an energy of $\epsilon \simeq 5$ is that of fig. 2 ; this shows little if any clustering. For a larger energy, $\epsilon \simeq 18$, there are clear signs of cluster formation (fig.3) and for an energy $\epsilon \simeq 36$ the cluster formation is dominant (fig.4). It is obvious from these figures, and those of Joyce and Montgomery, that clustering is a clearly observable phenomena, at least in the coulomb system. We hope that a more detailed examination of these and other numerical simulations, and their comparison with the theory presented here, will be given elsewhere.

ACKNOWLEDGEMENT

We would like to thank J.P. Christiansen for the calculations referred to above and for several useful discussions. We are also grateful to T. Martin for the numerical evaluation of equation 30.

REFERENCES

Christiansen, J.P. 1970 Culham Laboratory Report CLM R-106. London: H.M. Stationery Office.

Christiansen, J.P. and Taylor, J.B. 1973 Plasma Physics 15, 585.

Dawson, J., Okuda, H. and Carlile, R.N. 1971 Phys. Rev. Lett. 27, 491.

Edwards, S.F. 1958 Phil. Mag. 3, 119.

Hauge, E.H. and Hemmer, P.C., 1971 Physica Norvegica 5, 209.

Joyce, G. and Montgomery, D. 1973 J. Plasma Phys. (to appear)

Lee, Y.C. and Liu, C.S. 1973 Phys. Rev. Lett. 30, 361.

Lin, C.C. 1943 On the motion of Vortices in Two Dimensions. Toronto: University of Toronto Press.

Montgomery, D. 1972a Phys. Letters 39A, 7.

Montgomery, D. 1972b Phys. Letters 39A, 371.

Montgomery, D. 1972c Proc. Les Houches Summer School, Les Houches, France.

Montgomery, D. and Tappert, F. 1972 Phys. Fluids 15, 683.

Okuda, H. and Dawson, J. 1973 Phys Fluids 16, 408.

Onsager, L. 1949 Nuovo Cimento Suppl. 6 (9), 279.

Salzberg, A.M. and Prager, S. 1963 J. Chem. Phys. 38, 2587.

Taylor, J.B. 1972a Phys. Letters 40A, 1.

Taylor, J.B. 1972b Proc. 5th European Conf. on Controlled Fusion and Plasma Physics, Grenoble, France.

Taylor, J.B. and McNamara, B. 1971 Phys. Fluids 14, 1492.

Taylor, J.B. and Thompson, W.B. 1973 Phys. Fluids 16, 111.

Vahala, G. and Montgomery, D. 1971 J. Plasma Phys. 6, 425.

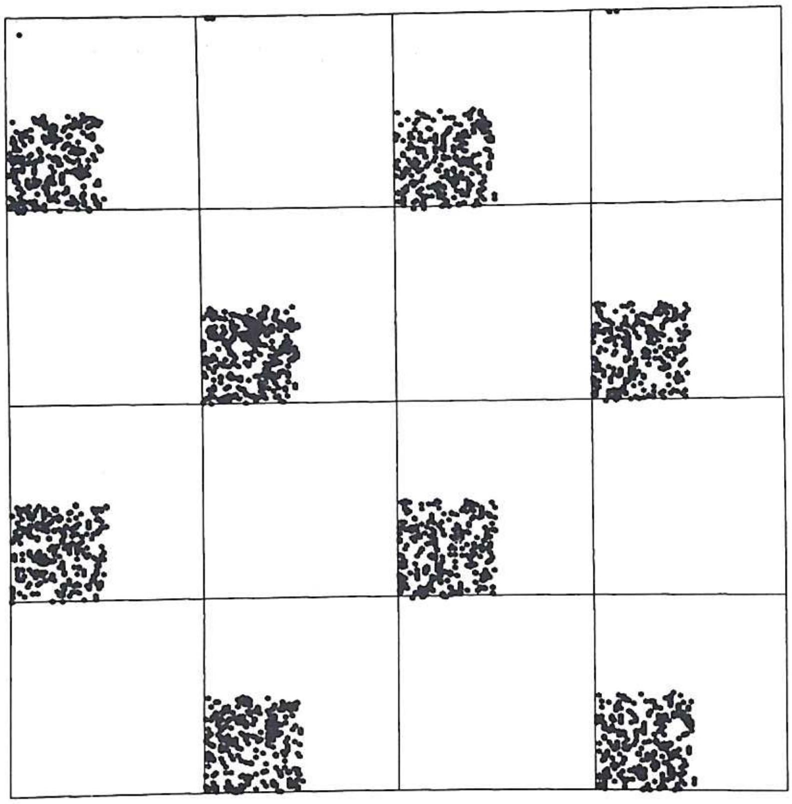

Fig.1. Typical Initial Distribution of Particles (Only positive particles shown)

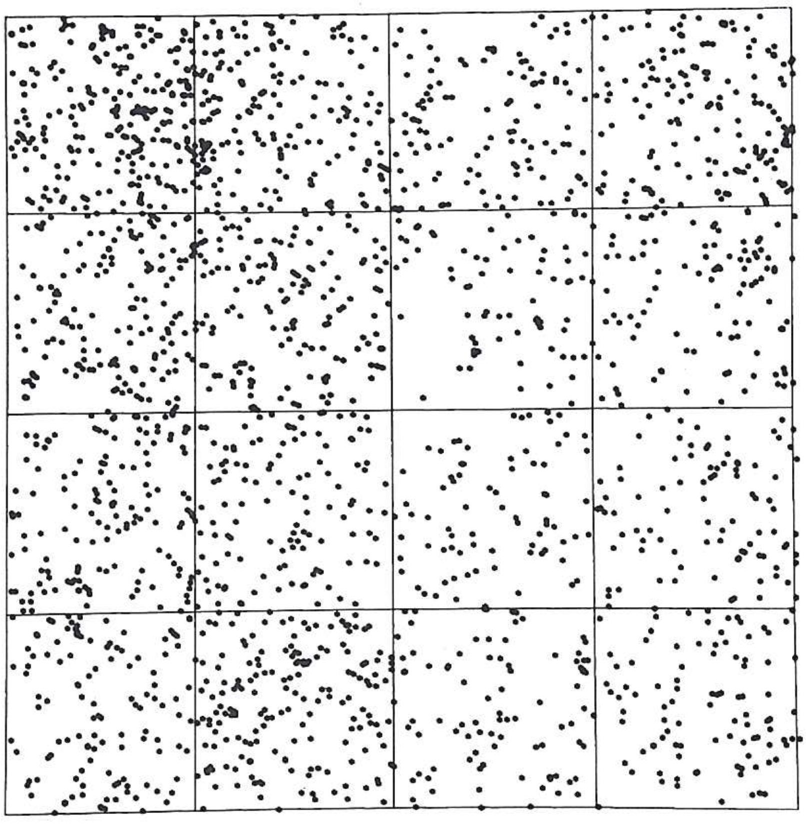

Fig.2. Typical Equilibrium Distribution — (Positive Particles, ϵ = 5)

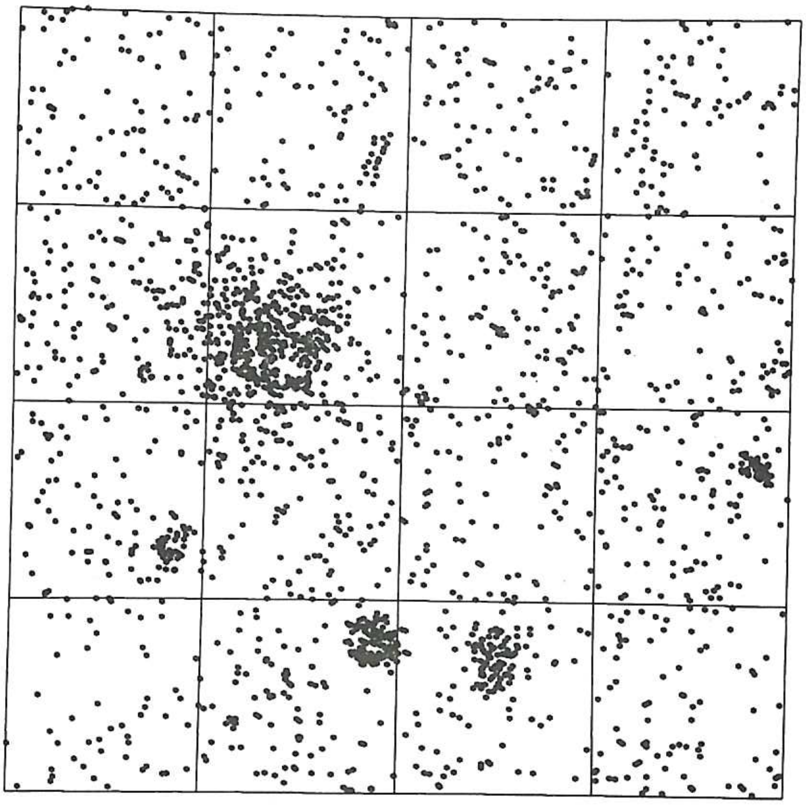

Fig.3. Typical Equilibrium Distribution — (Positive Particles, ϵ = 18)

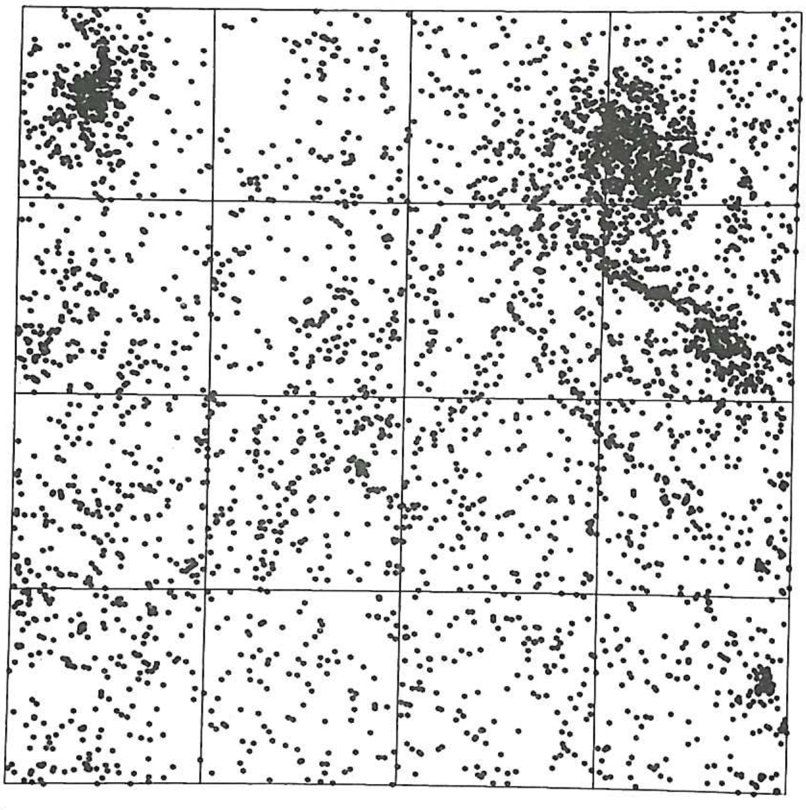

Fig.4. Typical Equilibrium Distribution — (Positive Particles, ϵ = 36)