Phase transitions in Euler fluids

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Phase transitions in two-dimensional (2D) Euler fluids are studied using mean field theory (MFT) solutions and Monte Carlo simulations. The MFT solutions show the possibility of first and second order phase transitions and the critical pointlike behavior. The simulations of the dynamics of 2D vortex patches agree with the MFT solutions over a wide range of parameters except at high energies where there are deviations between the two.

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Euler equations constitute a group of area preserving reparametrization of two-dimensional fluid motions. The long time states of these motions are often dominated by the presence of large scale coherent structures formed via inverse cascade of energy. Since the time of Onsager [1], statistical mechanical arguments have been used to explain these features. The basic idea is to approximate the continous vorticity field by a large but finite number of point vortices N and construct equilibrium measures within a bounded domain Ω. In such domains, the entropy S attains a maxima for a finite value of the total energy $W=\overline{W}$, so that for $W>\overline{W}$, the temperature $T=(\partial S/\partial W)^{-1}$ is formally negative. In this regime, the like sign vortices merge to give large vortex clusters. Though it was not proposed, Onsagar and others expected this description to be valid in the thermodynamic limit $N\rightarrow\infty$. Frohlich and Ruelle [2], who later examined the limit $N\rightarrow\infty$ for a neutral vortex gas, showed that it was not so, i.e., in the limit $N\rightarrow\infty$, $\overline{W}\rightarrow\infty$. Since the entropy dominates over the energy, all one obtains in this limit is a homogenous structureless equilibrium with trivial correlations. Another problem with the statistical mechanics of point vortices is that the description in terms of the canonical ensemble does not exist below a certain temperature [3]. In fact some authors [4] have argued that the microcanonical ensemble is the only appropriate ensemble for the vortex gas. This brings us to another peculiarity of the statistical mechanics of vortices, i.e., the nonequivalence of microcanonical and canonical ensembles.

Euler equations in two dimensions admit an infinite set of invariants that are smooth integrals of vorticity ω over the domain Ω. Part of the above stated difficulty is due to the fact that the statistical mechanics of point vortices do not respect the invariance of all these integrals. Miller *et al.* [5] and Robert and Sommeria [6] have recently shown that the infinite set of integrals, sometimes called the ''Casimirs invariants,'' can be included in the statistical description by dividing the domain Ω into N small squares of area a^2 containing a constant vorticity ω. By permuting local exchanges of vorticity between nearby boxes such that no two vortex patches overlap, these authors have constructed the canonical partition function that is a sum over a number of appropriate microstates. Some of the important consequences of this approach follow: First, the canonical ensemble is now well defined at all temperatures; second, by appropriate rescaling of the inverse temperature, i.e, $\beta=N\ \overline{\beta}$ where $\beta=T^{-1}$ and $\overline{\beta}$ is independent of N, the regime of negative temperature and the inhomogenous equilibria with nontrivial correlations is recovered in the limit $N\rightarrow\infty$; third, the mean field theory (MFT) that is the saddle point approximation to the canonical partition function becomes exact in the limit of vanishing discretization $a\rightarrow 0$, $N\rightarrow\infty$. The assumption of separation of scales is essential in this approach. Though one would expect the exactness of MFT on account of the long range nature of Coulomb interaction, there has been some debate on this point recently. The existence of the limit $\overline{\beta}=\lim_{N\rightarrow\infty}(\beta/N)$ has also been questioned by Chorin [7]. By numerically constructing the canonical partition function for the case of two species neutral vortex gas, it has been shown that this limit exists only for moderate values of temperatures and total energy W. One way to check the validity of the Miller-Robert mean field theory would be to numerically simulate the dynamics of an ensemble of vortex patches. Using the Metropolis algorithm this has been done by Miller *et al.* [5] for one-dimensional (1D) solutions of single species nonneutral vortex gas. But this is not enough. As is well known, above a certain energy, the maximum entropy solutions do not share the symmetry of 1D solutions. Smith [8] and Smith and O'Neil [9] have performed a Monte Carlo (MC) simulation for a collection of point vortices confined in a cylindrical geometry (r,θ) to examine the 1D to 2D transition. Later, Chen and Cross [10] undertook a more detailed study of the MFT solutions. It was shown that in some parameter space, the bifurcation of 1D to 2D solutions is subcritical giving rise to the possibility of discontinuous first order phase transitionlike jumps when β is used as the control parameter.

In this paper our task is twofold. First, by employing an efficient algorithm due to Turkington and Whittaker (TW) [11] we construct MFT solutions for arbitrary W and β. This algorithm is particularly useful for constructing MFT solutions with multiple spots. The phase-diagram of solutions confirms the possibility of first order phase transitions shown earlier by Chen and Cross. More importantly, these diagrams

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show the existence of a ''tricritical point'' (CP) in these systems. At this point, the second order phase transition curve passes into the first order phase transition curve [12] and the effective specific heat defined by $C_L = dW/d\beta|_L$ is infinite. First order phase transitions lead to the spontaneous formation of crystalline patterns of tight spots of vorticity. These crystalline patterns called, the ''vortex crystals,'' have recently been observed in the non-neutral plasma experiments [13]. Since the classic work of Thirring, Lynden-Bell, and Wood [14], such phase transitions involving clustering and fragmentation in the gravitational system are known and were discussed earlier. Also, the existence of the critical pointlike behavior in a system like the present one, which is governed by long range forces, is interesting from the point of view of ongoing debates about the nature of criticality in similar systems in 3D, i.e., ionic fluids (for details see Ref. [15]). In the second part of our paper, we perform extensive (MC) simulations of the dynamical evolution of an ensemble of vortex patches. The simulation has been performed with different numbers of patches, runlengths, and grid sizes, etc. We use the Metropolis algorithm for canonical and the Creutz algorithm for microcanonical simulations. Over a wide range of energies and β we find close agreement between the simulation and MFT solutions. However, at sufficiently large W we find deviations between the two solutions.

Following Miller *et al.* [5] and Robert and Sommeria [6] we consider an incompressible Euler flow in a simply connected domain Ω of the plane (x,y). All physical quantities are assumed dimensionless. The system is finite along $\hat{y}$ with boundary conditions at $y = \pm R/2$ and periodic along $\hat{x}$ with R as the periodic length. The evolution of this flow is described by velocity-vorticity equations given by

$$\omega_t + \mathbf{v}\cdot\boldsymbol{\nabla}\omega = 0, \quad \mathbf{v} = \boldsymbol{\nabla}\varphi \times \hat{\mathbf{z}}, \quad \nabla^2\varphi = -\omega. \tag{1}$$

Further, we consider an initial condition with two levels of ω such that within a fractional area α of total area A, $\omega = q$, while elsewhere $\omega = 0$. Thus the total circulation is $\Gamma = q\alpha A$. The entropy functional for self-avoiding dynamics is $S(\omega) = -\int d\mathbf{x}\ [\varrho \ln \varrho + (1-\varrho)\ln(1-\varrho)]$, where $\varrho = \omega(\mathbf{r})/q$. The statistical equilibrium of the flow under the constraint of total circulation $\Gamma = \int \omega\ d\mathbf{r}$, total energy $W = \frac{1}{2}\int \omega\varphi\ d\mathbf{r}$, and total linear momentum $L = \int y\omega\ d\mathbf{r}$ can be obtained by maximizing the entropy functional S given earlier and is given by [5,6]

$$\omega(\mathbf{r}) = \frac{q}{1+\exp(q\mu + q\beta\varphi + q\gamma\ y)}, \quad \nabla^2\varphi = -\omega, \tag{2}$$

where μ, β, and γ are the Lagrange multipliers. For given values of Γ, W, L, α, and the boundary conditions for φ at $y = \pm R/2$, $\varphi(x,y)$ and the values of μ, β, γ can be obtained by solving Eq. (2) along with the three constraints. These then are the mean field equations where μ, β, γ have been appropriately scaled with N [5]. In this form, the MFT preserves all the infinite invariants of the Euler equations. As stated earlier, MFT is the saddle point approximation to the partition function that, as argued by Miller *et al.*, becomes exact in the limit of vanishing discretization $a \to 0$. The vorticity distribution is stationary in a frame moving along $\hat{x}$ with a velocity γ. For y-symmetric boundary conditions $\varphi(x, y = \pm R/2) = 0$, $L = 0$. Solutions of Eq. (2) are constructed using a scheme due to Turkington and Whittaker [11] that relies on the fact that for $T < 0$, the entropy density is a concave function while the energy density is a convex function of $\varrho(\mathbf{r})$. As a result, the iteration procedure quickly converges to the solution with the desired number of vortices from an initial guess seeded with the same number of vortices. The solutions are constructed in a square box of size 4×4. The variational problem is considered solved if the (maximum) relative error between two successive iterations for $\varrho(\mathbf{r}), W$, and L is of the order $[1-5]\times 10^{-3}$. In Fig. 1 we plot the phase diagram in β-W space and show some solutions for a given value of L and for k_0, k_1, and k_2 ($k_n = 2\pi n/R$, $n = 0,1,2,\ldots$). Out of these $k_0 = 0$ corresponds to 1D (y-dependent) solution, while k_1 and k_2 are the 2D solution with 1 and 2 maxima of the vorticity, respectively. As shown in Fig. 1 and noted earlier [9] at $W = W_1$, there is a bifurcation from the k_0 to the k_1 branch. For $W > W_1$, the k_1 solution has higher entropy than k_0 solution. At higher energies there are bifurcations to k_2 and higher branches (not shown) that are local maximas of the entropy functional. In Fig. 2 we show the k_3 solution with three spots of concen-

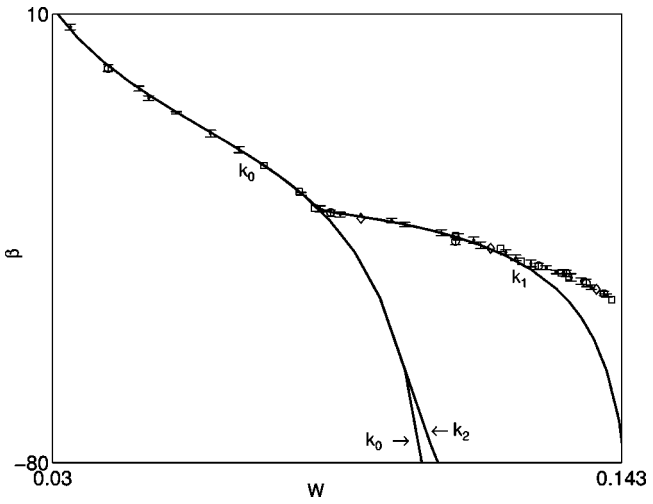

FIG. 1. β-W plots from the MFT and simulations for $\Gamma = 1$, $q = 1$, and $L = 0.4375$. The solid line is from MFT while ''points'' are from simulations as explained in the text.

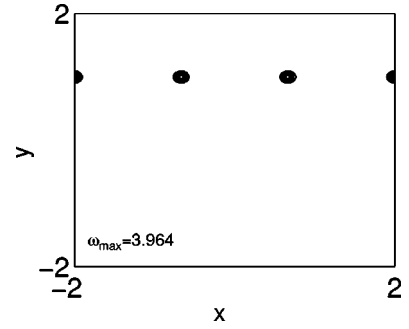

FIG. 2. The $n = 3$ solution on the high energy branch for $W = 4.6\times 10^{-3}$, $L = 0.2$, $\Gamma = 0.2$, and $q = 8$.

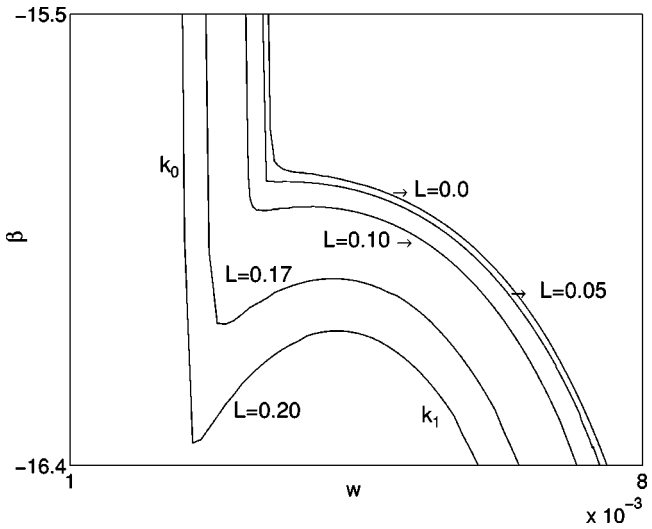

FIG. 3. β-W curves for the k_0 and k_1 branches for various values of L; $\Gamma=0.2$, and $q=8$.

trated vorticity. Except for the cylindrical geometry, this pattern is very similar to one of the ''vortex crystal'' patterns observed in the non-neutral plasma experiment [13].

Next, we turn to a discussion of the nature of phase transitions in these solutions. In Fig. 3 we plot the $k=k_0$ and k_1 branch for a number of L values using the TW algorithm. From these diagrams the following picture emerges.

(i) *First order phase transitions*. For large values of $L>L_c$ the specific heat C_L is negative in some range of W. This is also the range of L where the bifurcation is subcritical when β is used as the control parameter. Since, in the present model, the energy is bounded from above, the β-W curve turns around and $\beta\rightarrow-\infty$ as $W\rightarrow W_{max}$. As expected, in the range where $C_L<0$, the microcanonical and canonical ensemble differ from each other and, as noted by Chen and Cross [10], this can be attributed to the first order phase transition between 1D and 2D solutions. Since like sign vortices normally repel each other, one may find the presence of the first order phase transition in such system somewhat surprising. To understand this we recall Onsager's observation that the negative temperature regime is equivalent to a positive temperature regime with the opposite sign of the Hamiltonian and hence in this regime the like sign vortices attract each other. This provides the long range attraction between the vortices (and is responsible for $C_L<0$ in β-W curves). The incompressibility of patches, on the other hand, provides the short range hard corelike repulsion. Hence it is not surprising that such systems display first order phase transitions. In these transitions, concentrated spots of vorticity will be spontaneously formed. This has been observed in the experiments [13].

(ii) *Second order phase transitions*. For values of $L<L_c$ in Fig. 3, the bifurcation of $n=1$ solution from $n=0$ solution is supercritical or forward pitch fork when β is used as the control parameter. In these transitions, as one moves along an isotherm of L value$<L_c$, there is a continuous and smooth transition from the $n=0$ to the $n=1$ solutions. In this sense, these transitions may be termed as the second order phase transitions [10].

(iii) *Tricritical point of continuous transitions*. As is known, the second order phase transition curve in the PT plane segregates phases of different symmetry and hence does not terminate at some point. Rather, through this point, it passes into a curve of first order transitions. This point is called the CP of second order phase transitions and is analogous to an ordinary critical point [12]. This is exactly what happens in the present case. Along the critical isotherm $L=L_c$ in Fig. 3, second order phase transition curves ($L<L_c$) pass into first order phase transition curves ($L>L_c$). The L_c isotherm is locally flat at the point (β_c, W_c, L_c), where the specific heat $C_L=\infty$. This is the tricritical point of the k_1 branch and at this point in the β-L plane (not shown here], the first and second order phase transition curves will meet. Earlier, Smith and O'Neil [9] have studied the 1D to 2D bifurcation for point vortices and noted that it has signatures of the critical behavior, i.e., large persistent fluctuations and correlation lengths. However, one lacuna in this scenario, as noted by the authors themselves, is that on account of ''Kraichnan's collapse'' this behavior exists only in the microcanonical ensemble and not in the canonical ensemble. This is an unsatisfactory feature. In the present case this situation is ratified. Because of the hard core the collapse at low temperature is stabilized and the critical behavior and second order transitions exist in microcanonical as well as canonical ensembles. We will return to these points while discussing our simulation results.

In the second part of our work we have done extensive Monto Carlo simulations in order to check the validity of MFT results described above. For this purpose the domain of interest Ω of area $A=4\times4$ is divided into a large number of small patches, out of which N are filled. A move consists of exchange of vorticity between two randomly chosen sites. Such interactions are regarded as long range collisions. The calculations are performed by constructing an explicit Green's function for this geometry. For a given value of W, the initial condition is chosen by annealing. For the microcanonical ensemble the system interacts with a ''demon'' whose energy and momentum are restricted to a narrow range around given W and L. The value of β is obtained by fitting exponential functions to the frequency table of the demon. The simulation is done with 256, 512, and 1024, numbers of patches. The run lengths typically range from 30 000 to 50 000 steps. As patches are of finite size, an increase N corresponds to the refinement of the grid. In the microcanonical ensemble the lagrange multipliers are calculated for various runlengths 5000, 10 000, 15 000, and 20 000, etc. and $N=256$, 512, and 1024. In Fig. 1 we plot β obtained from simulations with W for fixed L. The error bars indicate fluctuations in β with run lengths, while the ''point and error bars'' are for $N=256$, ''circles and error bars'' are for $N=512$, and ''diamonds'' are for $N=1024$. In general, we find that there is nil, or very little, variation of β values with either N or run lengths. We find that it is adequate to use $N=256$ and run lengths of the order of 5000 MC steps. We attribute this feature of our MC to (a) the long range of the interaction, (b) the weak Coulomb singularity in 2D, and (c) short range cutoff due to finite size of the patch (which further weakens the singularity). For our canonical simula-

tion we employ a hybrid algorithm, i.e., microcanonical for momentum L and Metropolis for β. For comparison with MFT results we set β to values obtained from MFT and obtain the corresponding mean energies $\langle W \rangle$ that is plotted as W in Fig. 1. The canonical results are shown by points within the box.

Over a wide range of parameters we find a good agreement between MFT and simulations. In Fig. 3, if the system is taken along an isotherm with $L<L_c$, then both microcanonical and canonical simulations converge rapidly to the MFT solutions for all energies. In this sense, in our simulations one can go smoothly from 1D to 2D solutions as would be the case in the second order phase transitions.

As is evident from Fig. 1, at large energies we find deviations between simulation and MFT solutions. We have confirmed that this discrepancy appears both in microcanonical and canonical simulations and is independent of N and the grid size. These deviations seem to confirm Chorin's suspicion of the validity of MFT at large W (though he has demonstrated this for the case of neutral vortex gas). These deviations cast doubts on the quantitative accuracy of the first order phase transitions predicted by MFT where one phase lies on the high energy branch. Though we are unable to confirm it, we believe that our simulations will also exhibit Van der-Waal loops at high W. Due to deviations, these may be quantitatively different from the MFT loops. To see this, we recall that first order phase transitions require a short range repulsion and a long range attraction. Both these features are present in our simulation; as patches have finite size there is a short range hard corelike repulsion while in the negative temperature regime there is a long range attraction between patches. However, as said earlier, with practical problems related to available computing machines at our disposal, we are unable to do simulations in this regime. In any case, this is an interesting situation. As is known in systems with short range forces, the MFT gives a good description of the first order transition but fails near CP. In contrast, in the present system (which is governed by long range Coulomb force) it gives a good description of CP but fails to describe first order transition accurately.

To summarize, using the TW algorithm, we have constructed a phase diagram of solutions of the MFT. These solutions show the existence of the first and second order phase transition and the critical pointlike behavior in some parameter space. In the second part of our work we have performed extensive MC simulations of the dynamics of an ensemble of vortex patches. Over a wide range of parameters, MFT and simulations results agree with each other. However, at large W, there are deviations between the MFT and the simulation results.

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