Phase-Transition Behavior in a Negative-Temperature Guiding-Center Plasma

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The microcanonical ensemble of identical guiding centers in a two-dimensional, circular domain is characterized by means of a Monte Carlo simulation. For sufficiently large energies, the rotational symmetry is spontaneously broken so that a net displacement of the system accounts for a significant fraction of the angular momentum. The transition between axisymmetric and displaced statistical equilibria resembles a second-order phase transition. The description also applies to point vortices bounded by a circular equipotential surface.

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In this Letter I present numerical evidence of a qualitative change in the statistical equilibria of an isolated, cylindrically bounded system of two-dimensional guiding centers (i.e., line charges in a strong magnetic field), or point vortices in a two-dimensional fluid. Rotational symmetry is spontaneously broken at large energies, when the accessible region in phase space is dominated by configurations in which the particles form a single cluster away from the center of the domain. This breaking of a continuous symmetry is analogous to a second-order phase transition, in that thermodynamic derivatives are discontinuous and large relative fluctuations persist in the limit of many particles (although the system does not have a well-defined thermodynamic limit and the order parameter is not a local field). The transition occurs at a negative effective temperature, which is small enough that the system would collapse to a single point vortex if it were coupled to a heat bath. Hence the behavior of the canonical and microcanonical ensembles are qualitatively different.

Specifically, I consider N identical guiding centers with charge e, at positions $\{\mathbf{r}_i, i=1,\ldots,N\}$ confined in a conducting cylinder of radius R, parallel to a magnetic induction field $B\hat{\mathbf{z}}$. When B is large, inertia may be neglected. Hence the total canonical angular momentum, which is conserved because of rotational symmetry, is dominated by the magnetic vector potential contributions,[1] and so we write it as $P_\theta = -(eB/2c)\sum_i r_i^2$, where the sum is over particles. To leading order in $1/B$ the velocity of each guiding center is $\mathbf{v}_i = (c/B)\hat{\mathbf{z}}\times\nabla\phi(\mathbf{r}_i)$, where ϕ is the electrostatic potential due to other particles and the boundary charges, which are readily computed by the method of images. The equations of motion are Hamilton's equations for canonical coordinates proportional to the Cartesian coordinates of the guiding-center positions.[2-4] The Hamiltonian, which is proportional to the total electrostatic energy, is

$$H = \left(\frac{ec}{Bl}\right)\left[-\sum_{i\neq j}\ln\left(\frac{r_{ij}}{R}\right)+\frac{1}{2}\sum_{i,j}\ln\left(\frac{d_{ij}r_j}{R^2}\right)\right],$$

where l is the length along B over which charge is distributed, $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, and $d_{ij} = |\mathbf{r}_i - (R^2/r_j^2)\mathbf{r}_j|$. To make the analogy with point vortices, charge is interpreted as circulation and electrostatic potential as a stream function. Then P_θ is proportional to the kinetic angular momentum of the fluid and H to its kinetic energy. This particular system has been studied previously,[3,4] but the spontaneously broken symmetry appears to have been overlooked. (Related phenomena in other vortex guiding-center systems are discussed in Refs. 2, but without the present emphasis.) If we suppose that the energy and angular momentum are the only conserved quantities, and that evolution of the system is ergodic, then long-time averages should be statistically equivalent to averages over the microcanonical ensemble defined by fixed values E and M of the functions H and P_θ, respectively.

The model may apply to several physical systems. In the limit of large magnetic field and rapid equilibrium of motion along magnetic field lines, a non-neutral plasma confined in a circular cylindrical Penning trap[5] can be represented by two-dimensional guiding centers, for time scales long compared to the equilibration of the guiding-center positions, but short compared to the time for exchange of energy with velocity-space degrees of freedom. In particular, the model may describe states resulting from the nonlinear evolution of diocotron instabilities.[6] The vortex gas in statistical equilibrium has been used as a model for high-Reynolds-number, two-dimensional turbulence.[7,8] A similar model (with the sign of the energy reversed) could apply to self-gravitating matter, although the boundary conditions are somewhat artificial in that case.

Because of the long-range character of the Coulomb interaction, the energy scales with N^2, and thermodynamic quantities must be reinterpreted accordingly.[2] The entropy $S(E,M)$ is asymptotically proportional to N, and the inverse temperature, $\beta = \partial S/\partial E$, to $1/N$. It is also useful to define an effective rotation frequency $\omega = (1/\beta)\partial S/\partial M$, which is proportional to N; this quantity relates to the exchange of angular momentum with external systems, although it is *not* necessarily the local rotation rate of any part of the guiding-center system itself.[9] Hereafter energies will be normalized to e^2/l, length to R, and ω to $ec/2BR^2$. Since phase space is bounded, β is negative for large energies, as noted by Onsager.[7] There is an extensive literature on negative-temperature guiding-center and vortex systems, mostly concerned with the globally neutral, unbounded case (cf. Refs. 2-4 and 8). Most previous work has employed a weak-correlation approximation, leading to an equation for the mean density or one-particle spatial distribution function $n(\mathbf{r})$ which in this case is

$$n = n_0 \exp\{-\beta(-4\pi e^2 \nabla^{-2} n + \omega r^2)\}, \tag{1}$$

where the inverse Laplacian ∇^{-2} is defined with Dirichlet boundary conditions. A detailed exposition of the mean-field theory of the transition will be presented elsewhere.[9] The transition is associated with nonuniqueness of solutions to Eq. (1); a similar situation in a related problem is discussed in Refs. 4 and 10.

A simple argument suggests the possibility of displaced equilibria. Large energies correspond to the proximity of many particles. For fixed angular momentum, energetic axisymmetry equilibria would consist of a dense core and a halo of particles at large radii. Such a separation into two populations would decrease the mean-field entropy $(-\int d^2r\, n \ln n)$ compared to a single cluster displaced from the axis, and so the latter should be more likely. The transition is analogous to the condensation of density fluctuations into long wavelengths at large energies in other guiding-center or vortex configurations.[2,8]

I have tested the above picture with a series of numerical experiments. Creutz's[11] microcanonical Monte Carlo simulation technique was adapted to approximate the ensemble specified by given values of the energy, particle number, and angular momentum defined above. The degrees of freedom are $2N$ floating-point numbers, viz., N positions in a disk of unit radius. An initial configuration with energy E_0 and angular momentum M_0 is established (ordinarily by annealing a configuration saved from a previous run). The system is then coupled to a "demon" whose state is defined by an energy E_D and angular momentum M_D, lying in limited ranges, $|E_D| < E_M$, $|M_D| < M_M$. A candidate for a step to another configuration is constructed by using a pseudo-random-number generator to pick two distinct particle indices i and j, and displacements $\delta\mathbf{r}_i, \delta\mathbf{r}_j$ uniformly distributed on a square of edge length Δ. (Displacements which would leave the domain are rejected.) The changes in the energy and angular momentum associated with the displacements are computed; the new configuration is accepted if and only if these amounts can be transferred from the demon without exceeding its parameter ranges. Evolution of this sort of "long-range collision" between two particles is more efficient than single-particle moves, since it allows for more rapid radial motion consistent with the fixed value of the mean-square radius. (Some runs with one-particle moves were done to confirm that differences between ensemble averages based on the two schemes were equivalent, within statistical accuracy.) A "Monte Carlo step per particle," or MCS, consists of N such "collisions." The step scale Δ is adjusted to maintain a rejection ratio consistent with efficient exploration of phase space. Most of the data presented here were taken in runs of 40000 MCS at each value of energy and angular momentum. Although I have no proof that this algorithm accurately represents the microcanonical ensemble, the success of similar methods in other contexts[11,12] and the consistency with mean-field theory away from the transition are encouraging.

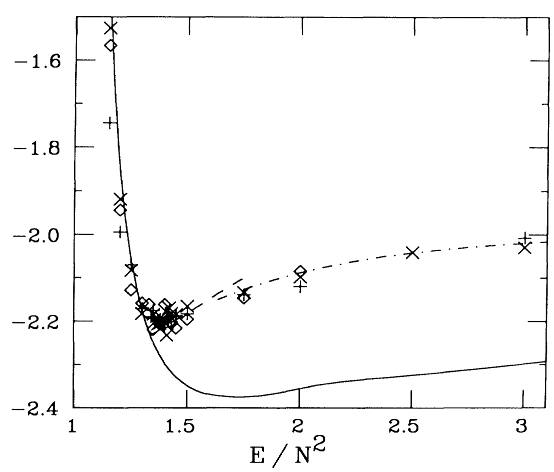

FIG. 1. Inverse temperature vs system energy. The angular momentum was fixed so that the mean-square radius was 0.1 ± 0.001. +, $N=256$; ×, $N=512$; ◇, $N=1024$. Solid line, axisymmetric solutions of Eq. (1); dashed line, near-critical behavior of displaced solutions to Eq. (1); dot-dashed line, asymptotic (large energy) behavior (Ref. 9). The mean-field critical energy is $1.338N^2$. Adjusted standard deviations: $N\delta\beta \approx 0.01$.

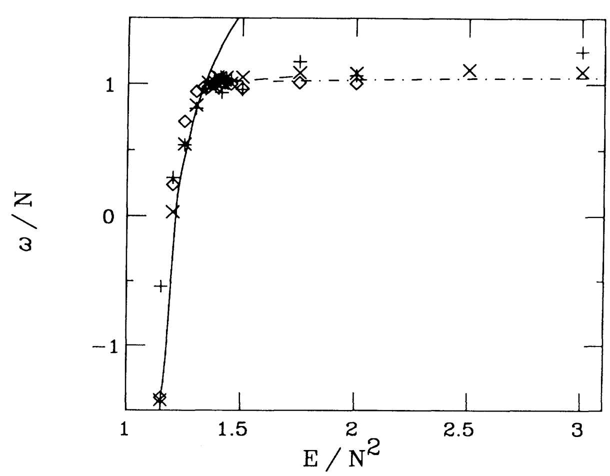

FIG. 2. Rotation frequency vs system energy. Symbols and parameters are as in Fig. 1. Adjusted standard deviations: $\delta\omega/N \approx 0.05$.

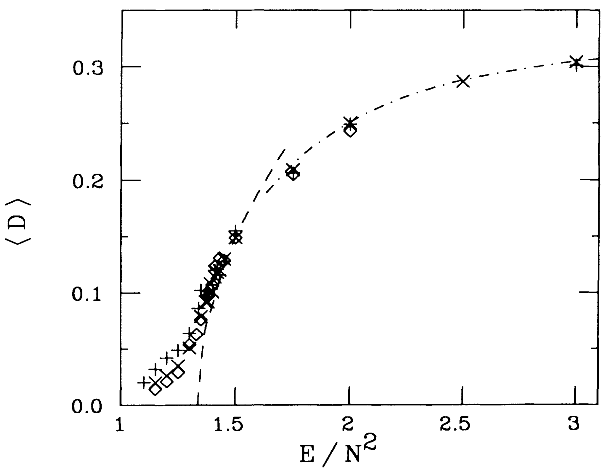

FIG. 3. Order parameter (average dipole moment) vs system energy. Symbols and parameters are as in Fig. 1. Adjusted standard deviations: $\delta D \approx 0.001$.

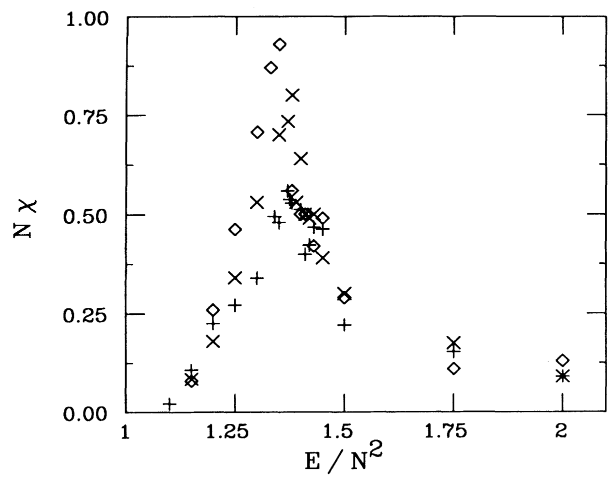

FIG. 4. Scaled susceptibility vs system energy. Symbols and parameters are as in Fig. 1. Adjusted standard deviations: $\delta\chi \approx 0.05\chi$.

As noted by Creutz, the demon is effectively in thermal equilibrium with a heat bath for large N, and its energy and angular momentum distributions tend to the forms $\exp\{-\beta E_D\}$ and $\exp\{-\beta\omega M_D\}$ accordingly. The temperature and rotation frequency determined from the demon distributions are shown as functions of energy in Figs. 1 and 2. The bounds E_M and M_M must be chosen small enough that the system parameters are accurately defined; this effectively limits the accuracy of β to about 1%, and that of ω to about 5% for the data shown. The relations deduced from the mean-field analysis[9] are also shown. The simulation results are consistent with axisymmetric solutions to Eq. (1) below the critical energy, and asymmetric solutions above. An argument of Kraichnan[8] shows that collapse should occur in the canonical ensemble for $N\beta < -2$, which applies to all the displaced equilibria observed in this study. This has been substantiated by the failure of a canonical Monte Carlo simulation to converge at such temperatures; at lower energies canonical and microcanonical simulations are consistent. Furthermore, thermodynamic instability under coupling to a heat bath is indicated by the negative specific heat $-\beta^2/(\partial\beta/\partial E)$ of the displaced phase. Axisymmetric equilibria with $N\beta < -2$, but energy below the critical value, are metastable states.

An appropriate order parameter, or measure of asymmetry, is the net dipole moment per particle $D = |\sum_i \mathbf{r}_i|/N$. (The modulus avoids difficulties associated with the ambiguity of direction.) In the non-neutral plasma, D is proportional to the amplitude of the fundamental diocotron mode. The dependence of ensemble averages of D on energy is indicated in Fig. 3. In the symmetric phase, $\langle D\rangle$ has a small value associated with thermal fluctuations and is approximately proportional to $1/\sqrt{N}$. In the displaced phase, $\langle D\rangle$ is nearly independent of N and grows slowly to the maximum value consistent with the prescribed mean-square radius. The statistical fluctuations of D are measured by $\chi = N|\beta|\langle(D-\langle D\rangle)^2\rangle$, which may be interpreted as a generalized susceptibility in the usual way. The scaled susceptibility $N\chi$, which is displayed in Fig. 4, shows no systematic dependence on N away from the critical regime, but increases roughly as $\sqrt{N}$ at the transition. As N increases, the locations of the peak in χ and of the minimum of β appear to converge to the critical energy of mean-field theory.[9]

Statistical errors in the data presented here are relatively large, because of correlations which persist over intervals of up to about 100 MCS. The error estimates given with Figs. 3 and 4 are corrected for these correlations, as described by Binder.[13] The correlations are presumably related to the long range of interaction, and are exacerbated by critical slowing down near the transition. The computational expense of high-quality statistics forbids any confident extraction of critical exponents using phenomenological finite-N scaling arguments[12] at this time.

The configurations which predominate in the high-energy phase are dynamical equilibria in a frame rotating at the frequency ω. The highest contours of the ensemble-averaged density (adjusted for the arbitrariness in azimuth) are localized away from the center of the domain; in the rotating frame, the mean flow follows the time-independent contours. The configuration is thus a special case of a finite-amplitude diocotron mode.[14] Analogous configurations in Penning traps have been shown to last for many rotation periods.[6] Further research will be needed to clarify the conditions for the validity of statistical equilibrium models for such experiments.

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