

Charge distribution in two-dimensional electrostatics

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Abstract

We examine the stability of ring-like configurations of N charges on a plane interacting through the potential $V(z_1, \dots, z_N) = \sum |z_i|^2 - \sum_{i < j} \ln |z_i - z_j|^2$. We interpret the equilibrium distributions in terms of a shell model and compare predictions of the model with the results of numerical simulations for systems with up to 100 particles.

Determining the distributions of charged particles in a central potential is a classic problem which has been studied since the nature of the electric force was first understood [1]. In two dimensions the Coulomb potential varies logarithmically with distance and describes, for example, the interaction of

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parallel charged wires. One could consider the physical problem of determining the electrostatic configuration of a group of parallel wires with like charges confined by a central force.

Ideas such as this have been applied to the description of the ‘crystalline state’ of cooled particle beams [2], where, in their rest frame, the beams are approximated by line-charges, and the central force, implemented by focusing magnets for example, is imposed to maintain the width of the beam. A similar situation arises in systems of charged particles where the dielectric properties of their environment are so highly anisotropic that the system is approximately two dimensional. An example is the the distribution of charged ions on superfluid surfaces. The Coulomb interactions in this system can be made effectively logarithmic and the crystalline states of the ions have been studied [3].

Another setting where Wigner crystal states are thought to play a role are the low density and high field states in the fractional quantum Hall system [4]. In the incompressible quantum fluid which exhibits the fractional quantum Hall effect, the ground state is described by Laughlin’s wavefunction [5,6]. At higher fields and lower densities of electrons, it is conjectured that the same system is in a Wigner crystal state. (This state has recently been observed experimentally [4].) There is the interesting question of whether there can be other states intermediate between a quantum Hall state and a Wigner crystal and whether these states could be described by a Laughlin-like wavefunction. It is not known to what extent Laughlin’s wavefunction continues to give a reasonable description of the electronic ground state for low densities and high fields.

We shall begin by studying the electrostatic problem of finding the configuration of particles which minimizes the potential energy

$$V(z_1, \dots, z_N) = \sum_{i=1}^N |z_i|^2 - \sum_{i<j} \ln |z_i - z_j|^2, \quad (1)$$

where z_i are the complex coordinates of particle positions in a plane. The central well is the interior potential of a uniformly charged disc. It obeys the Poisson equation $-\nabla^2 |z|^2 = -4$ so the background charge density is $-1/\pi$, independent of the radius of the disc. There is also a repulsive Coulombic (in two dimensions) interparticle potential. The potential (1) is the (suitably rescaled) logarithm of Laughlin’s wavefunction for the fractional quantum

Hall effect states [4,5]. The wavefunction is given by

$$\psi(z_1, \dots, z_N) = \prod_{i < j} (z_i - z_j)^\alpha \exp\left(-H \sum_i |z_i|^2/2\right)$$

and $\rho(z_1, \dots, z_N) = \psi^\dagger \psi = \exp[-\alpha V(\sqrt{H/2\alpha} z_i)]$, where H is the magnetic field and $\nu = 1/\alpha$ is the filling factor. For values of α and H relevant to the fractional quantum Hall effect the particle distribution and density correlations described by $\psi(z_1, \dots, z_N)$ are those of an incompressible liquid [6]. As α and H are increased there is a phase transition to a state where the probable distributions of particles described by $\psi(z_1, \dots, z_N)$ is concentrated at the classical minima of V . This is the analog of a crystalline state.

Let us begin with a simple mathematical problem. If we have a few particles in this system, we expect that they will lie on a ring at some equilibrium radius R . If we add more particles we expect that they increase the size of the ring to a maximum. An interesting question is: how large can the ring be before it is unstable? Also, even if the ring is stable to small oscillations, there is the more difficult question of whether it is actually a global minimum of the potential energy or whether there exist other, more favorable states.

The symmetry of the problem indicates that the configuration with N particles lying on the ring is a stationary point of the potential energy. To reason that a ring should have some maximum size where it is no longer a local minimum of the energy, consider the following continuum argument: Instead of point particles we allow the charge density to be continuous so that the energy is now given by

$$\begin{aligned} V[\rho] &= \int d^2z |z|^2 \rho(z) \\ &- \frac{1}{2} \int d^2z \int d^2z' \rho(z) \rho(z') \ln |z - z'|^2 \\ &+ \lambda \left(N - \int d^2z \rho(z) \right). \end{aligned}$$

Here λ is a Lagrange multiplier to fix the total charge. This potential is stationary where

$$|z|^2 - \int d^2z' \rho(z') \ln |z - z'|^2 - \lambda = 0, \quad \int d^2z \rho(z) = N.$$

These equations are solved by

$$\rho(z) = \begin{cases} 1/\pi, & |z| < R \\ 0, & |z| > R \end{cases} \quad \text{with } R^2 = N, \quad (2)$$

a uniform disc-shaped charge density (which, as expected, exactly compensates the background charge of the disc). Thus we expect that, in the limit of large numbers of particles, where we can approximate their distribution as continuous, the average of the distribution is uniform rather than ring-like and therefore large rings should be unstable unless they contain a sufficiently large charge in their interior.

In the following, we shall consider (and find an exact answer for) the slightly more general question of how large the ring can be when there is an azimuthally symmetric charge distribution inside. Such a configuration should minimize the energy

$$\begin{aligned} V_Q(z_1, \dots, z_N) &= \sum_i |z_i|^2 - \sum_{i < j} \ln |z_i - z_j|^2 \\ &+ \sum_i \int d^2 z' \ln |z_i - z'|^2 \rho(|z'|), \end{aligned} \quad (3)$$

where $\int_{|z'| < R} d^2 z' \rho(|z'|) = Q$.

The first variation of V_Q is

$$\begin{aligned} &\delta V_Q(z_1, \dots, z_N) \\ &= \sum_i (\bar{z}_i \delta z_i + \delta \bar{z}_i z_i) - \sum_{i < j} \left(\frac{\delta z_i - \delta z_j}{z_i - z_j} + \frac{\delta \bar{z}_i - \delta \bar{z}_j}{\bar{z}_i - \bar{z}_j} \right) \\ &- \sum_i \int d^2 z' \left(\frac{\delta z_i}{z_i - z'} + \frac{\delta \bar{z}_i}{\bar{z}_i - z'} \right) \rho(|z'|). \end{aligned} \quad (4)$$

We make the ansatz $z_k = R \exp(2\pi i k/N)$ for $k = 1, \dots, N$. This assumes that N particles sit on a ring which encloses an azimuthally symmetric charge distribution. Of course, if there are particles inside the ring, the charge distribution inside will not be azimuthally symmetric. However, especially in the limit of large numbers of particles, cancelling forces from approximately evenly distributed point charges should make this a good approximation.

From (4) we obtain the equation

$$R^2 = Q + \sum_{k=1}^N \frac{1}{1 - \exp(2\pi i k/N)} = Q + (N-1)/2, \quad (5)$$

where we have used the sum rule (A.2). Thus, we find that the ring configuration is always an *extremum* of the energy. In order to see whether it is a *local minimum* or a *saddle point* we must compute the eigenvalues of the stability matrix given by the second variation

$$\begin{aligned} & \delta^2 V_Q(z_1, \dots, z_N) \\ &= 2 \sum_k \delta \bar{z}_k z_k + \frac{1}{2} \sum_{j < k} \left(\frac{(\delta z_j - \delta z_k)^2}{(z_j - z_k)^2} + \frac{(\delta \bar{z}_j - \delta \bar{z}_k)^2}{(\bar{z}_j - \bar{z}_k)^2} \right) \\ &+ \sum_k \int d^2 z' \rho(|z'|) \left(\frac{\delta z_k \delta z_k}{(z_k - z')^2} + \frac{\delta \bar{z}_k \delta \bar{z}_k}{(\bar{z}_k - \bar{z}')^2} \right). \end{aligned} \quad (6)$$

Using the summation formula in equations (A.2) and (A.3), the parameterization of the equilibrium positions $\delta z_k = z_k (\delta \ln R_k + i \delta \phi_k)$, and the formula (5) for R^2 , we get

$$\begin{aligned} \delta^2 V_Q &= \sum_i \left(4Q + \frac{1}{6} (N-1)(11-N) \right) \delta \ln R_i \delta \ln R_i \\ &+ \frac{1}{2} \sum_{i \neq j} \frac{\delta \ln R_i \delta \ln R_j}{\sin^2 \pi(i-j)/N} + \sum_i \frac{1}{6} (N-1)^2 \delta \phi_i \delta \phi_i \\ &- \frac{1}{2} \sum_{i \neq j} \frac{\delta \phi_i \delta \phi_j}{\sin^2 \pi(i-j)/N}. \end{aligned} \quad (7)$$

The stability matrices are related to spectra of the Calogero model and can be diagonalized by techniques developed in Ref. 7 and reviewed in Appendix. For the angular fluctuations, $\delta \phi_i$, the spectrum is $s(N-s)$, $s = 0, \dots, N-1$, and for radial fluctuations, $\delta \ln R_i$ it is $4Q + 2(N-1) - s(N-s)$, $s = 0, \dots, N-1$. The angular modes are non-negative, indicating stability to angular fluctuations for all N . The zero mode for $s = 0$ is a consequence of rotation invariance of V_Q . For large enough N some radial modes are negative, indicating instability of the radial fluctuations. The minimum of the radial spectrum occurs at $s = N/2$ (if N is even). The maximum value of N for which this minimum is positive is the largest integer less than

$$N_{\max} = 4 \left(\sqrt{Q + 1/2} + 1 \right). \quad (8)$$

For a system with a total of $M = N + Q$ particles, the largest number which will lie on the outside ring is given by the largest integer less than

$$N_{\max} = 4 \left(\sqrt{M + 1/2} - 1 \right). \quad (9)$$

It is interesting to note that, as particles are added to a ring, the first mode of instability to radial fluctuations appears for the mode of maximum frequency, i.e. that where every second particle moves inward and the other particles move outward. Locally, instead of the ring rejecting the last particle and forcing it to the center of the distribution, its first tendency is to split into two rings of roughly equal size.

A numerical calculation using simulated annealing Monte Carlo methods can be used to find the equilibrium distribution of the particles for N up to 100. The result is that, to a good approximation, particles lie on concentric rings with the number of particles per ring increasing like the square root of the radius of the ring and with average spatial density close to the value $1/\pi$ given in (2).

The structure that we see is reminiscent of the shell model of the atom. We can devise a model for predicting the number of particles in each ring. We begin by using Eq.(9) to calculate the maximum number of particles which fit in the outer ring, which depends on the total number of particles. Then we subtract that number from the total and compute how many particles will fit in the next ring given the total remaining number of particles and so on until the total number of particles is exhausted. This gives the maximum occupation numbers of concentric rings.

There are two limits to the accuracy of this model. First, the internal charge distribution is approximated as azimuthally symmetric, rather than distributed at points. In the real system the rings are perturbed by the inhomogeneities of the charge distribution and are not exactly circular. We expect that azimuthal symmetry is a good approximation when the number of particles is large. Second, the model is accurate only when each ring tends to fill to its locally stable configuration with maximum number of particles. In almost every case, this is unlikely as there can be many preferred, lower energy states where rings are not filled to maximum capacity.

We know that this already happens for a six particles. Our theoretical computation indicates that six particles sitting on the corners of a hexagon is stable to small perturbations. However, explicit calculation reveals that the configuration with five particles sitting on corners of a pentagon with a single particle at the center is also stable to perturbations and has slightly lower energy than the hexagon. Therefore, already for six particles our shell model is approximate.

It is then interesting to ask how accurate it is for higher numbers of particles. Some results of a numerical simulations compared with predictions

of the shell model are

M :	2	3	4	5	6	7	8	9	10	15	25	100
N_{exp} :	2	3	4	5	5/1	6/1	7/1	7/2	8/2	11/4	14/9/2	31/25/19/14/8/3
N_{th} :	2	3	4	5	6	6/1	7/1	8/1	8/2	11/4	16/8/1	36/28/20/12/4

where, for both the experimental and theoretical values we also denote the number of particles in the inner rings, starting from the largest. We see qualitative agreement of the results of the model. However quantitative predictions are reliable only within about 30%. Also, since the rings do not fill to their maximum, we tend to underestimate the number of rings¹. We also estimate the accuracy of the computer simulation itself to be within about two or three for the population of the rings. (This estimate is obtained from reproducibility of the results.)

The shells are generally not filled to their maximum population since global minima of the potential appear first. It would be interesting to obtain a ring-filling criterion which sought global minima of the energy. This would be an analog of Hund's rule for filling of electronic orbitals in atoms [8]. We haven't yet succeeded in doing this, our only present recourse is to explicit calculations and comparisons of the total energy of different configurations of a few particles and numerical simulations.

As a test of the accuracy of the shell model, we have used a numerical simulation to find the equilibrium configurations in the region between 40 and 60 particles. Below we show the number and population of the rings observed and compare with the numbers and populations of rings which are computed using the shell model,

M :	40	41	42	43	44	45
N_{th} :	21/13/6	21/14/6	22/14/6	22/14/6/1	22/14/7/1	22/15/7/1
N_{exp} :	19/14/6/1	19/13/7/2	18/15/7/2	20/13/8/2	21/15/7/1	20/14/8/3

M :	46	47	48	49	50
N_{th} :	23/15/7/1	23/15/8/1	23/16/8/1	24/16/8/1	24/16/8/2
N_{exp} :	21/14/9/2	21/13/10/3	21/14/9/4	20/14/9/5/1	22/15/9/4

M :	51	52	53	54	55
N_{th} :	24/16/9/2	24/17/9/2	25/17/9/2	25/17/10/2	25/18/10/2
N_{exp} :	21/16/8/5/1	22/15/9/5/1	22/15/10/5/1	22/16/11/5	21/17/10/6/1

¹ The computer simulation of the 100 particle case is shown in Fig.1, see the original paper

M :	56	57	58	59	60
N_{th} :	26/18/10/2	26/18/10/3	26/18/11/3	26/19/11/3	27/19/11/3
N_{exp} :	23/17/9/6/1	22/17/11/6/1	22/17/11/6/2	23/15/12/5/4	24/16/12/7/1

Experience shows that these numerical calculations are good to within plus or minus two or three particles per ring. The main source of error is distortion of the ring by inhomogeneities of the charge distribution. This is particularly acute for rings with near maximum numbers of particles. We see that our model predicts the population of the outer shell within 20% and gives reasonable populations for the inner shells.

Thus we see that the shell model describes well the qualitative, and approximately the quantitative properties of the frozen state of N particles up to 100 or so.

In conclusion, we observe that, even in the case of 100 particles², there is no observable tendency for the systems we study by numerical simulations to form a triangular Wigner crystal. The latter is the expected ground state in the limit of large numbers of particles. For a system which is too small, the tendency to form a regular crystalline state is frustrated by the boundary geometry. For large systems, this should be offset by two effects: First, the boundary energy grows more slowly than the bulk energy (the ratio is $1/\sqrt{M}$) so eventually the boundary should adjust itself to help minimize the energy of the bulk. Second, the effects of the boundary on particle positions well inside the bulk should be negligible because of the screening of the long-ranged Coulomb force by the gas of charged particles themselves. The screening length in a classical Coulomb gas is generally a few average spacings.

It is a mystery to us that we do not see the onset of Wigner crystallization. We might speculate about possible glass-like or quasi-crystalline phases of the system and perhaps a phase transition to other states as we increase the particle number. (Phase transitions are possible in this system with a finite number of degrees of freedom because it is classical - there is no tunneling which could restore a broken symmetry.) One idea which supports this speculation is the fact that, for six particles, the configuration with a pentagon and one particle in the center is preferred to a hexagon. Thus, locally the system may have a tendency to form structures with five-fold symmetry. However, this structure cannot form a lattice and so perhaps forms a frustrated state with no long-range order. This possibility is the subject of ongoing investigation.

² shown in Fig.1, see the original paper

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Appendix. The summations and diagonalizations of matrices used in this paper have been presented previously in the context of the Calogero model [7]. We shall summarize the technique in this Appendix. Consider the matrix $L_{jk} = (1 - \delta_{jk}) \{1 + i \cot \pi(j - k)/N\}$. We can show explicitly that the vector $\psi_k^s = \exp(-2\pi i k s/N)$, $s, k = 1, \dots, N$, is an eigenvector of L , i.e.,

$$\begin{aligned} & \sum_{k=0, k \neq j}^{N-1} (1 + i \cot \pi(j - k)/N) \exp(-2\pi i k s/N) \\ = & \exp(-2\pi i j s/N) \left(\sum_{k=1}^{N-1} \frac{-2 \exp((2s + 1)\pi i k/N)}{\exp(i\pi k/N) - \exp(-i\pi k/N)} \right), \quad (\text{A.1}) \end{aligned}$$

where we have combined the terms in (A.1) and changed variables $k \rightarrow j - k$ in the sum. After some algebra, the right-hand side of (A.1) is

$$- \left(\sum_{l=0}^{2s-2} \sum_{k=1}^{N-1} \exp[(2\pi i k/N)(l - s + 1)] \right).$$

The eigenvalue can further be written as

$$\sum_{l=0}^{2s-2} \left(1 - \sum_{k=1}^N \exp[(2\pi i k/N)(l - s + 1)] \right) = 2s - N - 1.$$

Thus, the eigenvalues of L are $2s - N - 1$, $s = 0, \dots, N$.

Next, we use the trigonometric identity

$$\cot \alpha \cot \beta = 1 - (\cot \alpha - \cot \beta) \cot(\alpha - \beta)$$

to show that

$$B = \frac{1}{2} \left(L^2 + 2L - \frac{1}{3} (n^2 - 1)I \right),$$

where

$$B_{jk} = (1 - \delta_{jk}) \left[1/\sin^2 \pi(j - k)/N \right].$$

This gives the eigenvalues of the matrix B as $\frac{1}{2}(N^2 - 1) - 2s(N - s)$, $s = 1, \dots, N$ which are used in Eq.(7) to get the spectra of small oscillations. The eigenvalue equation (A.1) also gives the sum rule

$$\sum_{k=1}^{N-1} \frac{\exp(-2\pi i k s / N)}{1 - \exp(2\pi i k / N)} = s - \frac{1}{2}(N + 1). \quad (\text{A.2})$$

Another sum rule can be derived from the eigenvalue equation for matrix B ,

$$\sum_{k=1}^{N-1} \frac{\cos 2k s \pi / N}{\sin^2 k \pi / N} = \frac{1}{3}(N^2 - 1) - 2s(N - s). \quad (\text{A.3})$$

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