

## Boundary Effects on Structures in Two Dimensional Dipolar Systems

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*Boundary induced perturbation in the ordering of two dimensional dipolar systems confined by a circular hard wall has been studied using Molecular Dynamics simulations. A pronounced shell-like structure is observed near the circular boundary. As expected, the structure away from the walls has hexagonal symmetry. The variance of average nearest neighbor distance,  $\Delta a/a$ , is extracted from our simulations. A quantitative comparison is made with recent experimental results on the structures of floating magnetic particles.*

### INTRODUCTION

Recently, there has been growing interest in physical systems demonstrating self-assembly behavior<sup>1</sup>. Much of the interest is motivated by the potential these systems show for the fabrication of photonic band gap crystals<sup>2</sup>, and much progress has been made in this area. Some of the important remaining issues are tunability of the band gap, ability to grow 3D photonic crystals, and perfection of the underlying lattice which, in turn, controls the gap density of states. Golosovsky et al<sup>2</sup> have studied most of these issues in their recent work with 2D arrays of magnetic particles floating on water. However, boundary induced disorder of the resulting lattice structure is not yet fully understood. To this end, we use Molecular Dynamics simulations to predict the resulting lattice structures of 2D dipoles and compare our predicted structures with observed configurations of magnetic particles. Values of  $a$  and  $\Delta a/a$  are extracted from the simulations and compared to those measured for floating magnetic particles. We use the complex bond orientational parameter,  $\psi_N$ <sup>3</sup>, and a radial density function to quantify boundary induced perturbations.

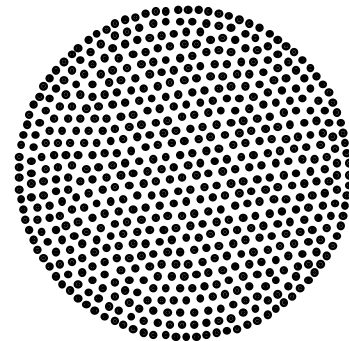
### METHOD

A Molecular Dynamics code written in C++, running on a Pentium processor and incorporating a small velocity dependant damping term was used to determine the equilibrium states of an  $n$ -body system,  $60 < n < 600$ , interacting via dipole-dipole potential in 2D. The magnetic degrees of freedom were fully constrained, i.e. perpendicular to the plane.

### RESULTS AND DISCUSSION

Numerous self-assembling systems with long range repulsive interactions are known to exhibit hexagonal

ordering within the bulk, when they are confined to a fixed volume. Magnetic bubbles in garnet films<sup>4</sup>, two-dimensional colloidal suspensions<sup>5</sup>, and floating magnetic particles<sup>2</sup> are a few examples. Fig. 1 below shows a typical result of our Molecular Dynamics simulation for an equilibrium configuration of 600 dipoles confined by a circular hard wall of radius 20 cm.



**Fig. 1:** Molecular Dynamics simulation of 600 dipoles

Apart from the expected hexagonal ordering in the bulk, Fig. 1 also illustrates that the structure near the boundary is shell-like. This seems to be imposed upon the system by the hard wall circular boundary. These shell-like structures have been explored in recent theoretical studies of melting in two dimensions<sup>6,7</sup>. However, in the context of tunable photonic crystals, boundary effects have not been fully explored. Our predicted structures (Fig 1 above) are in detailed and excellent agreement with the experimental results of Golosovsky et al<sup>2</sup>.

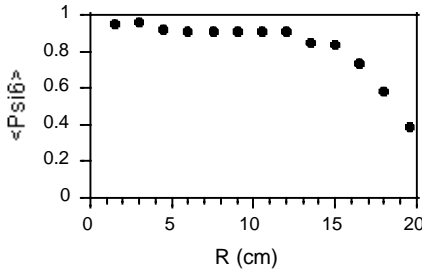
In the following, we present results we believe to be new. From our simulated structures, we extract  $\Delta a$ , the rms fluctuation of the nearest neighbor distance.  $\Delta a/a$  is a measure of the disorder of the structure and is of great practical concern because it affects the gap density of

states and therefor the usefulness of this structure for photonics applications. Our simulations for  $N = 61$  yield  $\Delta a/a$  ranging from 3% to 5% depending upon starting configurations etc. This is comparable to the experimentally observed values of about 10% for  $N = 61$  by Golosovsky et al<sup>2</sup>. The slightly larger experimental values suggest that the experimental system was subject to additional disorder, over and above what is caused by the circular boundary. Non-uniformity of the dipole moment is a likely candidate for this additional disorder, and we plan to explore this in future studies.

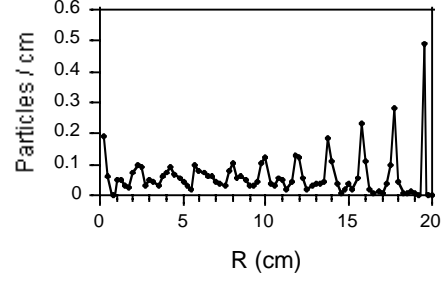
Because the dipole-dipole interaction varies as inverse cube of particle separation, there is no natural length scale in the problem which might determine the range over which boundary induced perturbations might heal as one moves away from the boundary, into the bulk. Our simulations appear to be consistent with the experimental data which suggests that  $\Delta a/a$  decreases rather slowly away from the boundary. In order to address this important question, we present the radial dependence of two measures of local order. The complex parameter,  $\psi_N$ , measures bond orientational order and is defined at discreet points by

$$\psi_N(r_{jk}) = \frac{1}{N} \sum_{j=1}^N e^{iN\theta_{jk}}$$

where  $N$  is the number of nearest neighbors and  $\theta_{jk}$  is the angle made with respect to a fixed axis by a segment connecting particle  $j$  to its  $k^{\text{th}}$  nearest neighbor. For sites with perfect  $N$ -fold coordination,  $\psi_N = 1$ . For sites with less than perfect coordination,  $\psi_N < 1$ . Here, we are concerned with hexagonal orientation, i.e.  $\psi_6$ . In four separate simulations of 325 particles, the value of  $\psi_6$  was computed for each particle and local average values of  $\psi_6$  were calculated. Figure 2 shows a plot of  $\langle \psi_6(R) \rangle$  vs.  $R$ , where the brackets indicate an average over all particles within a region.



**Fig 2:** Locally averaged  $\langle \psi_6(R) \rangle$



**Fig. 3:** Radial density distribution

A systematic decay in  $\langle \psi_6(R) \rangle$  is clearly observed near the boundary, but the quality of the data is not good enough to unambiguously determine the  $R$  dependence of  $\langle \psi_6(R) \rangle$ .

The boundary induced shell-like structures can be captured by constructing a binned average radial particle density function  $\rho(R)$ . One expects sharp peaks in  $\rho(R)$  near the boundary, which should broaden as one moves away from the boundary. This is evident in our calculated values of  $\rho(R)$ , shown in Fig. 3 above. It is reassuring to find in our simulations that the length scale over which  $\rho(R)$  decays away from the circular boundary is very close to the length scale over which  $\langle \psi_6(R) \rangle$  increases away from the boundary.

A systematic investigation of the dependence of  $\rho(R)$  and  $\langle \psi_6(R) \rangle$  upon different parameters therefore promises to be a fruitful direction for future research.

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