Ground State of Magnetic Dipoles on a Two-Dimensional Lattice: Structural Phases in Complex Plasmas

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We study analytically and by molecular dynamics simulations the ground state configuration of a system of magnetic dipoles fixed on a two-dimensional lattice. We find different phases, in close agreement with previous results. Building on this result and on the minimum energy requirement we determine the equilibrium lattice configuration, the magnetic order (ferromagnetic versus antiferromagnetic), and the magnetic polarization direction of a system of charged mesoscopic particles with magnetic dipole moments, in the domain where the strong electrostatic coupling leads to a crystalline ground state. Orders of magnitudes of the parameters of the system relevant to possible future dusty plasma experiments are discussed.

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There have been extensive studies on the properties of arrays of interacting dipoles fixed on lattice sites since the seminal work of Luttinger and Tisza in 1946 [1–3]. Subsequent investigations of two-dimensional (2D) lattices of interacting magnetic dipoles have been directed toward surface adsorbates [4–6] and thin magnetic films (TMF) [7]. These systems can be modeled as consisting of microscopic magnetic dipoles considered as 2D classical vectors that can rotate within the plane of the lattice [8] and interact via both exchange and classical dipole-dipole potentials.

Recent experiments in complex (dusty) plasmas have demonstrated that 2D lattices of charged, micron-sized dust grains can be levitated and confined in the sheath region of a plasma discharge [9,10]. Experiments on 2D colloidal suspensions have studied systems of paramagnetic particles on a liquid-gas interface, as well [11]. These experiments point to the emerging possibility of creating and studying lattices composed of charged grains with permanent magnetic dipole moments, as a macroscopic classical analog of TMF systems without exchange interaction.

In this Letter, we present results of a theoretical analysis accompanied by molecular dynamics (MD) simulations that lead us to the determination of the ground state configuration of such systems. We proceed in two steps. First we analyze systems of magnetic dipoles fixed on sites of a given 2D lattice that interact solely via the magnetic dipole-dipole potential. We recover earlier results by Rozenbaum [4] (see also [12]) pertaining to the ground state of dipoles on an arbitrary 2D Bravais lattice. Second, we address a scenario in a complex plasma, where the magnetic interaction competes with the dominant screened electrostatic Yukawa interaction between the grains, $\phi(r) = (Q^2/r)e^{-\kappa r}$ (with the inverse screening length κ), in the domain where the strong electrostatic coupling leads to a crystalline ground state [13–15]. The actual equilibrium lattice configuration is that which minimizes the combined electrostatic and magnetic dipole-dipole interaction energy of the system. The ultimate objective of this work is to find this equilibrium configuration as a function of the relative strengths of these two interactions. The strength of the magnetic interaction can be characterized by the magnetic coupling, $\Gamma_m = \mu^2/a^3 k_B T$, where μ is the magnetic moment of a grain, a is the Wigner-Seitz radius, $a = (1/n\pi)^{1/2}$, n is the density, and a relates to the square lattice constant and hexagonal lattice constant as follows: $a = a_{\text{square}}/\sqrt{\pi} = a_{\text{hex}}/\sqrt{2\pi/\sqrt{3}}$. The strength of the electrostatic interaction is given by the conventional plasma coupling parameter, $\Gamma = Z^2 e^2/a k_B T$ (Z is the charge state of a grain) and κ. The ratio $\eta = \Gamma_m/\Gamma$ is the important parameter on which to focus.

We begin by fixing the dipoles on a lattice and ask how the magnetic moments will order. This problem was treated analytically for an infinite lattice by Rozenbaum who approximated the dipole lattice sums by assuming that the ground state energy is dominated by the intrachain interactions. We assume a finite lattice, in keeping with the reality of a 2D plasma setup. Our results are in close agreement with [4].

The configuration of dipoles in a 2D lattice is partly determined by the symmetry of the lattice whose sites they occupy. We explore the full family of 2D Bravais lattices that can be characterized by two parameters, which fully describe the (generally rhombic) unit cell and can be chosen as the rhombic angle, denoted by ϕ, and the aspect ratio of the two sides of the rhomboid, denoted by ν.

Ignoring thermal excitation ($\Gamma_m \to \infty$) the ground state energy is the classical magnetic dipole pair energy summed over the entire lattice of dipoles:

$$\mathcal{E}_{\text{magnetic}} = \frac{1}{2}\sum_{ij} \frac{a^3}{r^3}[\vec{\mu}_i \cdot \vec{\mu}_j - 3(\vec{\mu}_i \cdot \hat{r})(\vec{\mu}_j \cdot \hat{r})], \quad (1)$$

where $\vec{r} \equiv |\vec{r}_i - \vec{r}_j|$ and $\vec{\mu}_i(\alpha)$ is the magnetic dipole moment vector of the ith particle, which for the purpose of this calculation may be taken as a unit vector. We measure r in units of a, thus rendering $\mathcal{E}_{\text{magnetic}}$ dimensionless. Equation (1) is still ill-defined as long as the magnetic phase and the orientation of the dipoles are not specified. Both of these depend on the lattice structure and are determined by the minimization of the interaction energy for a given lattice. A configuration where the dipoles point out of the plane of the lattice always has a higher energy than the one with all the dipoles lying in the lattice plane. Thus it is sufficient to consider the in-plane configurations.

In earlier studies [5] it was revealed that depending on the rhombic angle the equilibrium alignment can be either ferromagnetic (F) (as for the hexagonal lattice, $\phi = 60°$) or antiferromagnetic (AF) (as for the rectangular lattice, $\phi = 90°$). Focusing now on the F phase, we determine the equilibrium direction of the dipole orientations (i.e., the direction of the magnetization) by finding the ground state energy extrema with respect to magnetization direction α. This can be obtained analytically by minimizing the magnetic energy with respect to α, at a constant density. In Fig. 1 the dependence of the preferred F magnetization direction on ϕ and ν is shown. These results can be compared with those of [5]. Also shown in Fig. 1 are values generated by MD simulation, as explained below. Note that the mere existence of an optimum α for a given ϕ and ν does not ensure that in equilibrium the system is in the F phase at that rhombic angle: the state may be only metastable (as also explained below in relation to the MD simulation).

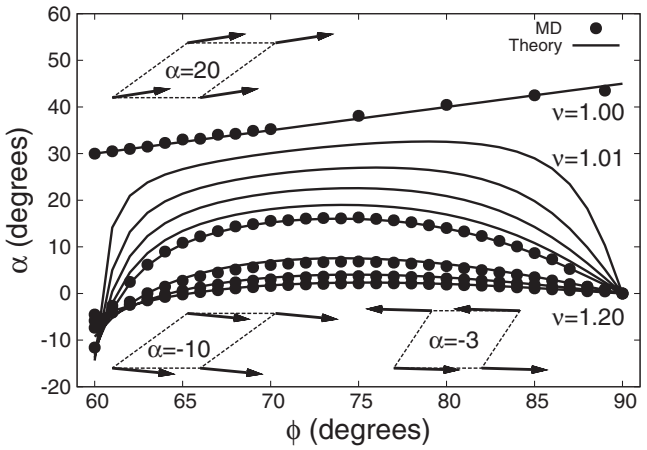

FIG. 1. Equilibrium F magnetization angles α versus the rhombic angle ϕ for a series of aspect ratios ν. Compared are theoretical results derived from equation (lines) and MD results for $\nu = 1.00$, 1.05, 1.10, 1.15, and 1.20 (points). Also shown are samples of different lattice and magnetic configurations. α is the angle that the dipole moments make with the x axis. In the AF case, the dipoles alternate being above and below the x axis (results not shown).

For $\nu = 1$ and $\phi = 60°$ (hexagonal lattice), at zero temperature the ground state is continuously degenerate with respect to the magnetization direction. However, this point seems to represent a singularity in the parameter space. For $\nu = 1$ and $\phi \neq 60$, for $\nu \neq 1$ for all ϕ, and for nonzero temperature [16] the degeneracy is removed. In the first case, for $\nu = 1$, the theoretically preferred magnetization direction is always $\alpha = \phi/2$ (the next-nearest neighbor direction), approaching $\alpha = 30°$ as $\phi \to 60°$. In the second case, however, for $\phi = 60°$, $\alpha \to -15°$ as $\nu \to 1$ (see Fig. 1). Interestingly, it was shown some time ago [16] that the degeneracy would also be removed at nonzero temperatures by thermal disorder even at $\phi = 60°$.

A calculation along the same lines has been performed for the optimum α in the AF phase. In the rectangular lattice ($\phi = 90°$) the alternating dipoles are in the $\alpha = 0°$ and $\alpha = 180°$ direction (columnar arrangement); for $\phi < 90°$, there is a small ν-dependent deviation from the columnar alignment (see Fig. 1). These results are not displayed in detail, because the largest deviation is less than 3°. At the singular point $\nu = 1$, $\phi = 90°$ the system again exhibits a continuous (vortical) degeneracy, as discovered by [17]. However, similar to the F case, this degeneracy is removed at other ϕ or ν values and by thermal disorder [16]. Some examples of the internal field configurations both in the F and in the AF phase are portrayed in Fig. 2: observe the formation of neutral points both in the F and AF phases.

The equilibrium value of α determines the actual interaction energy. These energies are plotted versus ϕ in Fig. 3. The intersection of the F and AF curves for a given value of ν indicates the critical rhombic angle ϕ_{crit} where a phase transition between the two configurations may take place. For $\phi < \phi_{\text{crit}}$ the ground state is the F phase, while for $\phi > \phi_{\text{crit}}$ the ground state is the AF phase. As shown in the

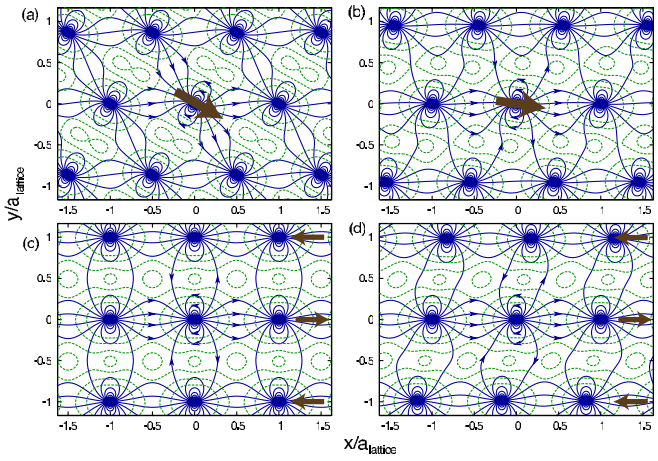

FIG. 2 (color online). Magnetic field lines and equi-B contours for F and AF configurations: (a) F, $\phi = 60°$, $\nu = 1.0$ (b) F, $\phi = 60°$, $\nu = 1.1$ (c) AF, $\phi = 90°$, $\nu = 1.0$, (d) AF, $\phi = 80°$, $\nu = 1.0$. Note the formation of neutral points in all cases. The arrows show the direction of magnetization.

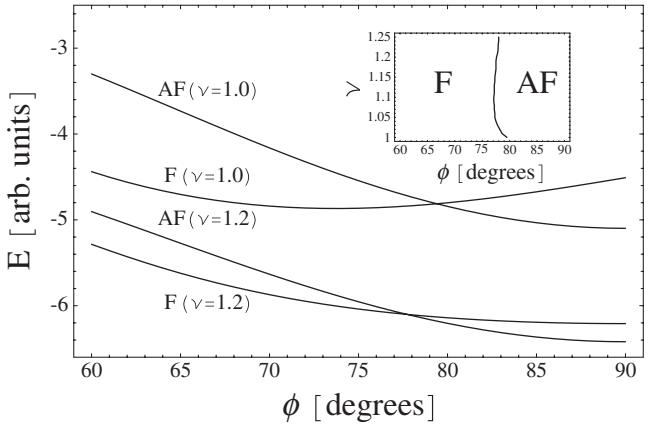

FIG. 3. Lattice energies due to the magnetic dipole pair interaction [Eq. (1)] only versus the rhombic angle ϕ for F and AF alignments at two values of the aspect ratio, $\nu = 1.0$ and $\nu = 1.2$. The crossings of the curves correspond to the F-AF phase transition. The inset shows the $\phi_{\rm crit}(\nu)$ phase boundary in the ϕ, ν parameter space.

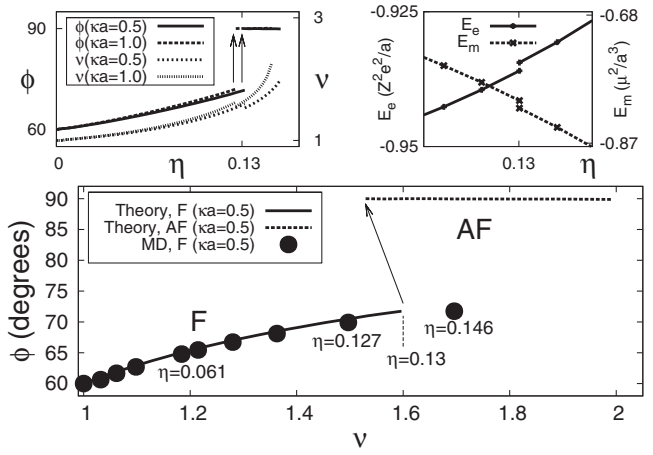

FIG. 4. Equilibrium lattice configurations in the ϕ, ν parameter space for different values of η at $\kappa a = 0.5$. In the upper panels the effect of increasing η on the rhombic angle ϕ and on the electric E_e and magnetic E_m interaction energies are shown (in E_e only the correlational part is indicated). Note the discontinuities in E_e and E_m at $\eta_{\rm crit} \simeq 0.13$; the total energy, however, changes continuously.

inset, $\phi_{\rm crit}$ is a slowly varying function of ν, with a value in the vicinity of 78°.

We proceed to consider a 2D complex plasma layer of negatively charged grains that each have a magnetic dipole moment. The electrostatic interaction acts as a repulsive force, keeping the particles apart, and competes with the magnetic interaction in determining the equilibrium lattice structure. As in the previous discussion, the density n is kept constant for all calculations.

The total energy, $E_{\rm total}$, is the sum of the electrostatic energy of the charges and the magnetic energy of the dipoles: $E_{\rm total} = \frac{Z^2e^2}{a}[\frac{1}{2}\sum_{ij}\frac{a}{r}e^{-\kappa r} + \eta\mathcal{E}_{\rm magnetic}]$, where the parameter η has been defined above. η is generally less than 1. For $\eta = 0$ the system is in a hexagonal configuration, $\phi = 60°$ and $\nu = 1.0$. However, it is well known that the electrostatic energy difference between the hexagonal and other lattice structures is very small [18,19]. Therefore even for small nonzero values of η the system will deform and assume a lattice configuration more preferable for the magnetic interaction energy. In order to find this configuration for a given set of κ and η values, a local minimum in the total energy is searched for in the (ϕ, ν) parameter space. Based on the previous results we expect that if $\phi <\approx 78°$, the system will be in the F phase, and if $\phi >\approx 78°$, the system will be in the AF phase. Indeed, this is borne out by our results. In Fig. 4 the detailed phase diagram versus ϕ, ν, and η is displayed. The plot shows that for $\kappa a = 0.5$ the system undergoes a first order transition from the F phase to the AF phase with an accompanying structural phase transition from a rhombic to a rectangular lattice at $\eta \simeq 0.13$. Increasing (decreasing) κ would result in slightly lower (higher) $\eta_{\rm crit}$ values. The magnetization directions are not shown in Fig. 4, but can be obtained from the previously determined dependence on the lattice configuration (ϕ and ν) (see Fig. 1).

In an experimental scenario, the magnetic dipole moment of a grain is determined by N_B, the number of aligned Bohr magnetons per grain. We assume that N_B is 10% of the number of atoms in the grain. For a sphere of iron with radius $R = 4$ μm, we estimate $N_B \simeq 1.3 \times 10^{12}$. The charge state of the sphere in an Ar plasma with electron temperature $\simeq 2$ eV is $Z \simeq 10^4$. With a lattice spacing of about 100 μm the value of $\eta \simeq 0.15$ is high enough for the phase transition to take place. It may be triggered by changing the density, n (since η is proportional to n), which in turn may be accomplished by relaxing or enhancing the confining electric potential. The signature of the F/AF transition would be the disappearance of the magnetic moment. One experimental concern may be the possible coalescence of the grains due to the dominance of the attractive dipole interaction at small distances. In order to avoid this scenario, one would require that the position, r, of the potential maximum between neighboring grains be at a distance $r < 2R$. A way to satisfy this condition would be by using particles with a small magnetic core $R_{\rm core} < R$. In this case a dust grain with $R \simeq 10$ μm and $R_{\rm core} \simeq 4$ μm may be appropriate. In order to have $\eta \simeq 0.13$ for a system composed of such dust grains would require that $a \simeq 25$ μm.

One might ask whether the magnetized electrons will diamagnetically screen the dipole-dipole interaction, or if the magnetization will affect the charging of the grains. However, with a typical magnetic field strength of 1.6 G at a distance of 25 μm from the grain the electron gyro frequency ω_L would be $\sim 3 \times 10^7$ rad/s, which can be compared with the electron-neutral collision frequency $\nu_{\rm en} \sim 3 \times 10^8$ s^{-1} under usual experimental conditions ($P = 0.5$ mbar, $T_e \sim 2$ eV); $\omega_L/\nu_{\rm en} \ll 1$ then shows the electrons to be relatively unaffected by the magnetic field.

Under low pressure conditions this may not be the case, but even then the electronic gyro radius (~ 2 cm) is too large to significantly alter the domination of the electron motion by the electric field.

All of our theoretical calculations have been carefully checked through computer simulations. The simulations follow the MD method from [20] (modified for a system with both translational and rotational degrees of freedom), using a rhombic simulation box and periodic boundary condition. The simulations were done at constant volume, which is appropriate for low temperatures. Only particle pairs separated by less than a cutoff radius R_{cut} are taken into account in the force and torque calculation in the solution of the equation of motion. At the beginning of the simulations the $N = 1600$ to 10 000 particles are placed at rhombic lattice sites with random angular velocities and velocities sampled from Maxwellian distributions. The computer experiments are performed after a proper thermalization, when the system has settled in an equilibrium state.

For the pure dipole system simulations are performed to investigate the equilibrium configurations, where only rotation is allowed. During the initial thermalization, the system is slowly cooled from $\Gamma_m = 1$ to 1000. Our results confirm the theoretical value of the critical rhombic angle $\phi_{\mathrm{crit}} \simeq 78^\circ$ for the phase boundary between the F and the AF state. However, due to the long relaxation times simulation of the F phase can continue well beyond 78° in a metastable state (see Fig. 1), characterized by discrete F domains and interacting domain walls featuring vortices. When started in the AF phase, the MD simulations can reproduce the fully ordered ground state configurations more easily. In the full 2D complex plasma simulation the particles are charged and free to move. The system is started in the F phase with sufficiently low temperature to allow small angle oscillations only. To find the ground state lattice parameters we compute the σ stress tensor in every time step. During the computation the simulation box is slowly transformed (adjusting ν and ϕ) in order to fulfill the stability conditions $\sigma_{xx} = \sigma_{yy}$ and $\sigma_{xy} = \sigma_{yx} = 0$, which defines the equilibrium lattice geometry. As shown in Figs. 1 and 4, the simulation results are in excellent agreement with theoretical predictions.

In summary, we have mapped, through analytic and MD methods, the phase diagram of the ground state configurations for a system of classical magnetic dipoles fixed on the sites of a 2D Bravais lattice. The appearance of F and AF phases and the variation of the direction of the magnetization as functions of the parameters ϕ (rhombic angle) and ν (aspect ratio) that characterize the lattice structure are the hallmarks of the combined effect of the electrostatic and magnetic interactions. We have considered the realization of such systems as 2D complex plasmas of mesoscopic charged particles also carrying a classical magnetic dipole moment. At sufficiently strong values of the electrostatic coupling a plasma crystal forms whose lattice structure and the concomitant magnetic order are determined by the competition of the relative strength η of the magnetic interaction to the electrostatic interaction: it is shown that at a critical value of η a structural phase transition from a rhombic to a rectangular lattice occurs, accompanied by a magnetic transition from the F phase to an AF phase. For the Yukawa screening parameter $\kappa a = 0.5$, $\eta_{\mathrm{crit}} = 0.13$ has been found. Experiments on plasma crystals within the desired parameter ranges seem to be feasible: confirming the theoretical predictions and further investigating the remarkable physics of such systems would be of great interest.

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[1] J. M. Luttinger and L. Tisza, Phys. Rev. **70**, 954 (1946).
[2] M. E. Fisher and A. Aharony, Phys. Rev. Lett. **30**, 559 (1973).
[3] A. Aharony and M. E. Fisher, Phys. Rev. B **8**, 3323 (1973).
[4] V. M. Rozenbaum, Zh. Eksp. Teor. Fiz. **99**, 1836 (1991) [Sov. Phys. JETP **72**, 1028 (1991)].
[5] V. M. Rozenbaum, V. M. Ogenko, and A. A. Chuiko, Sov. Phys. Usp. **34**, 883 (1991).
[6] V. M. Rozenbaum, Phys. Rev. B **53**, 6240 (1996).
[7] K. DeBell, A. B. MacIsaac, I. N. Booth, and J. P. Whitehead, Phys. Rev. B **55**, 15 108 (1997).
[8] E. Rastelli, S. Regina, A. Tassi, and A. Carbognani, Phys. Rev. B **65**, 094412 (2002).
[9] S. Nunomura, N. Ohno, and S. Takamura, Phys. Plasmas **5**, 3517 (1998).
[10] J. C. Reyes, M. Benesh, C. Chan, and T. W. Hyde, in Proceedings of the 49th Annual Meeting of the Division of Plasma Physics, Orlando, Florida, November 2007 (unpublished).
[11] K. Zahn, R. Lenke, and G. Maret, Phys. Rev. Lett. **82**, 2721 (1999).
[12] J. G. Brankov and D. M. Danchev, Physica (Amsterdam) **144A**, 128 (1987).
[13] J. H. Chu and I. Lin, Phys. Rev. Lett. **72**, 4009 (1994).
[14] H. Thomas, G. E. Morfill, V. Demmel, J. Goree, B. Feuerbacher, and D. Mohlmann, Phys. Rev. Lett. **73**, 652 (1994).
[15] V. E. Fortov, A. V. Ivlev, S. A. Khrapak, A. G. Khrapak, and G. E. Morfill, Phys. Rep. **421**, 1 (2005).
[16] C. Henley, Phys. Rev. Lett. **62**, 2056 (1989).
[17] P. Belobrov, S. Gekht, and V. Ignatchenko, Zh. Eksp. Teor. Fiz. **84**, 1097 (1983) [Sov. Phys. JETP **57**, 636 (1983)].
[18] F. M. Peeters and X. Wu, Phys. Rev. A **35**, 3109 (1987).
[19] L. Bonsall and A. Maradudin, Phys. Rev. B **15**, 1959 (1977).
[20] D. Frenkel and B. Smit, *Understanding Molecular Simulation* (Academic Press, New York, 1996).