Patterns of Striped Order in the Classical Lattice Coulomb Gas

Sung Jong Lee,[1] Jong-Rim Lee,[2] and Bongsoo Kim[3]

[1]*Department of Physics, The University of Suwon, Hwasung-Gun, Kyunggi-Do 445-743, Korea*

[2]*Division of Electronics, Computer and Telecommunications Engineering, Pukyong National University, Pusan 608-737, Korea*

[3]*Department of Physics, Changwon National University, Changwon 641-773, Korea*

(Received 23 April 2001; published 26 December 2001)

We obtain via Monte Carlo simulations the low-temperature charge configurations in the lattice Coulomb gas on a square lattice for charge filling ratio f in the range $1/3 < f < 1/2$. We find a simple regularity in the low-temperature charge configurations which consist of a suitable periodic combination of a few basic striped patterns characterized by the existence of partially filled diagonal channels. In general, there exist two separate transitions where the lower temperature transition (T_p) corresponds to the freezing of charges within the partially filled channels. T_p is found to be sensitively dependent on f through the charge number density $\nu = p_1/q_1$ within the channels.

DOI: 10.1103/PhysRevLett.88.025701 PACS numbers: 64.70.Rh, 64.60.Cn

The question of what would happen to a physical system, as the ratio between two competing physical parameters or scales is varied from a simple low order rational fraction to complicated higher order rational or even irrational limit, has been, for a long time, one of the important issues in diverse areas of physics in general and condensed matter physics in particular. Here, we focus our attention to the problem of finding the ground states for systems with a competition between periodic pinning potential and repulsive interparticle interactions, where interesting commensuration-incommensuration effects are expected to occur [1–3] as the particle filling density (playing the role of the above-mentioned ratio) is continuously varied. Typical experimental examples include monolayers of adsorbed atoms on crystalline substrates [4], and vortex systems under periodic pinning potentials such as Josephson junction arrays under uniform magnetic fields [5].

More specifically, in this work, we are dealing with the two-dimensional lattice Coulomb gas (LCG) which is one of the extensively studied model systems, where a fraction $f = p/q$ (p and q are relative primes) of the lattice sites are occupied by unit charges upon a uniform neutralizing background [6]. LCG appears in the vortex representation [7] of the two-dimensional Josephson junction arrays under uniform external magnetic field that are also represented as uniformly frustrated XY (UFXY) models [8]. In spite of many years of research effort, there still remains a wide range of f (notably $1/3 < f < 1/2$) for which not much is known in terms of equilibrium properties. Even the ground state configurations are known only for some limited values of f [9]. In this paper, we report, based on Monte Carlo (MC) simulations, the first systematic enumeration of the low-temperature ordered patterns of LCG on a square lattice for $1/3 < f < 1/2$.

In the case of a UFXY model on a square lattice, Halsey proposed staircase states [10] as the low-temperature ordered configurations with a $q \times q$ periodic unit cell. However, the staircase state turns out to be the true ground state for some limited values of f only such as $f = 1/2, 1/3, 2/5, 3/8$, etc. More recent works on a UFXY model [11,12] and LCG [13] show that, for $f = p/q$ near $1 - g(g = (\sqrt{5} - 1)/2)$ with q large, the low-temperature vortex configurations in the UFXY model can be different from the ordered charge configurations in LCG. Especially, in the case of LCG on a square lattice, it was shown [13] that there appear diagonal striped configurations with partially filled diagonals. However, the exact patterns of order at low-temperature for arbitrary values of f in the dense regime have not been enumerated yet.

In this paper, we find numerically that, for a large part of the range $1/3 < f < 1/2$, the ordered configuration consists of periodic arrangements of a few basic striped patterns. Four regimes of values of f are identified, each of which represents a specific class of striped patterns characterized by the existence of partially filled diagonals. The transition temperature T_c is found to be only weakly dependent on f. Below T_c, there exists a temperature range where the charges within partially filled diagonal channels are disordered (thus mobile along channels). We found that there exists another transition at a lower temperature T_p at which freezing of charges within partially filled channels occurs. This lower transition temperature depends sensitively on the rationality of the charge number density within channels $\nu = p_1/q_1$, decreasing monotonically in q_1.

General 2D LCG [14] is described by the following Hamiltonian:

$$\mathcal{H}_{\mathrm{CG}} = \frac{1}{2} \sum_{ij} Q_i G(\vec{r}_{ij}) Q_j \,, \tag{1}$$

where $\vec{r}_{ij}$ is the distance between the sites i and j, and the magnitude of charge Q_i at site i can take either $1 - f$ or $-f$. Charge neutrality condition $\sum_i Q_i = 0$ implies that the number density of the positive charges is equal to f. We can thus view the system as a lattice gas of

$N \cdot f$ charges of unit magnitude upon uniform negative background charges of charge density $-f$ ($N = L^2$ is the total size of the system with the linear dimension L). The lattice Green function $G(\vec{r}_{ij})$ solves the equation $(\Delta^2 - \lambda^{-2})G(\vec{r}_{ij}) = -2\pi\delta_{\vec{r}_{ij},0}$, where Δ^2 is the discrete lattice Laplacian and λ is the screening length. For the case of usual Villain transformation of the UFXY model, we have $\lambda = \infty$. But the screening term is included in this equation for generality. On a square lattice with periodic boundary conditions, $G(\vec{r})$ is given by

$$G(\vec{r}) = \frac{\pi}{N} \sum_{\vec{k}\neq 0} \frac{e^{i\vec{k}\cdot\vec{r}} - 1}{2 - \cos k_x - \cos k_y + 1/\lambda^2}, \qquad (2)$$

where $\vec{k}$ are the allowed wave vectors with $k_\mu = 2\pi n_\mu / L$ ($\mu = x, y$), with $n_\mu = 0, 1, \ldots, L-1$. In the case of infinite screening length, for large separation r, one gets $G(\vec{r}) \simeq -\ln r$ [14]. In this work, the presented results are all obtained for the case of $\lambda \to \infty$ [15].

In our MC simulations, the initial disordered random configuration is updated according to the standard Metropolis algorithm by selecting a positive charge at random and trial-moving it over to one of the *nearest neighbor* or *next nearest neighbor* sites [13].

Figure 1 shows the four basic component patterns. First, component pattern (I) is a sequence of three diagonals which are *empty, filled,* and *empty,* respectively [that may be denoted by (**010**) in our notation where **1** refers to a filled diagonal and **0** refers to an empty diagonal]. In other words, it is a pattern with a single isolated diagonal which is filled with charges, that is neighbored by empty diagonals on both sides. Repetition of this pattern generates the ground state configuration for $f = 1/3$.

Second, component pattern (II) consists of a sequence of five diagonals that can be written as (**01010**). This forms the basis of the ground state configuration for $f = 2/5$ with lattice periodicity five. The third component pattern (III) consists of a sequence of seven diagonals that can be denoted by (**010p010**), where **p** refers to a partially filled diagonal where only part of the diagonal sites are occupied by positive charges. This structure, which may be termed as a *channel* structure, can form a basis of a periodic configuration with spatial periodicity seven. Last, the fourth component pattern (IV) can be denoted by (**01010p01010**). This thick channel structure can form a basis of a periodic configuration with periodicity eleven.

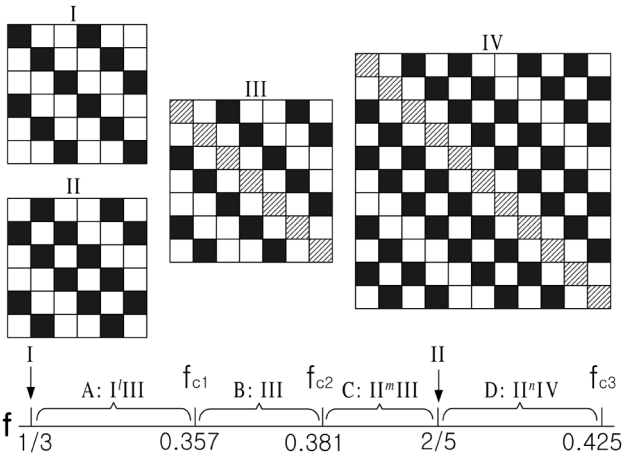

FIG. 1. Regimes of charge patterns for the range of value of f between 1/3 and 0.425. Filled squares and empty squares represent positive ($Q = 1 - f$) and negative ($Q = -f$) charges, respectively, while gray squares denote lattice sites forming partially filled diagonal channels, where only finite fraction ν of the sites are filled with positive charges.

We are now able to give a detailed description of the low-temperature charge patterns. We may identify four regimes for the striped charge configuration. We will call these by regimes A, B, C, and D respectively. Figure 2 shows typical representative configurations in each of the four regimes.

In regime A that is bounded by $1/3 \lesssim f \lesssim f_{c1}$ ($f_{c1} \simeq 0.357$), the low-temperature charge configuration consists of combinations of type I and III patterns, where l ($l = 1, 2, 3, \ldots$) copies of type I patterns in sequence followed by a single type III pattern ($\mathrm{I}^l\mathrm{III}$) form a basic unit, repetition of which forms the whole charge configuration. We can see that the lattice periodicity of the ordered stripe configuration is equal to $p_A = 3l + 7$. As the value of f increases within regime A, the value of l decreases in a steplike manner. Therefore, regime A is further divided into subregimes, each of which is characterized by a positive integer l.

Regime B covers the region $f_{c1} \lesssim f \lesssim f_{c2}$ ($f_{c2} \simeq 0.381$), where the ordered charge configuration simply consists of repetitions of type III stripe patterns with the resulting lattice periodicity $p_B = 7$. In regime C, which is bounded by $f_{c2} < f < 2/5$, the low-temperature charge

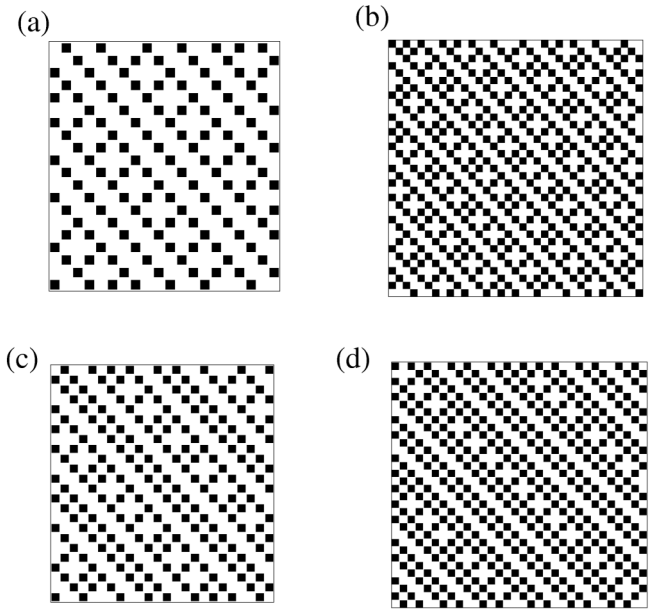

FIG. 2. Low-temperature charge configurations for (a) regime A with $f = 7/20$ ($l = 1$), (b) regime B with $f = 13/35$, (c) regime C with $f = 0.384$ ($m = 1$), and (d) regime D with $f = 0.41$ ($n = 1$), respectively.

configuration consists of combinations of type II and III patterns, with m ($m = 1, 2, 3, \ldots$) copies of type II stripe patterns in sequence followed by a single type III pattern ($\mathrm{II}^m\mathrm{III}$) forming a basic unit. Here, we can see that the lattice periodicity of the ordered stripe configuration is equal to $p_C = 5m + 7$. As the value of f increases within regime C, the value of m increases monotonically in a step-like manner.

Regime D corresponds to $2/5 < f \lesssim f_{c3}$ ($f_{c3} \simeq 0.425$), where the unit period of ordered configuration consists of combinations of a type IV pattern plus n ($n = 0, 1, 2, 3, \ldots$) repetitions of type II stripe patterns that may be denoted by $\mathrm{II}^n\mathrm{IV}$. We see that the periodicity of the striped order in regime IV is equal to $p_D = 5n + 11$.

The above results are all based on extensive Monte Carlo simulations. Beginning with random initial charge configurations, approximately 10^5 to 10^7 MC sweeps (depending on f) were performed at temperatures usually between $T = 0.025$ and $T = 0.03$ which are a little below the transition temperatures. For each of the four regimes, we checked five to ten different values of f for the simulations depending on the specific regime. We could identify the stripe periodicity p_S of the (potentially) stable charge configuration through tedious trial simulations (see also below). After that, in order to further make sure that we indeed found the stable configuration, we performed simulations with lattices of dimensions $2p_S \times 2p_S$, up to $6p_S \times 6p_S$. By this procedure, we could confirm that the above patterns are stable ones except for the extreme limiting situations mentioned below.

We could also determine the crossover densities, f_{c1}, f_{c2}, and f_{c3} by performing extensive Monte Carlo simulations. In addition, we were also guided by the following relations among f, ν (filling density inside the partially filled channels) and l, m, n that read $f = (l + 2 + \nu)/(3l + 7)$ (for regime A and B), $f = (2m + 2 + \nu)/(5m + 7)$ (regime C), and $f = (2n + 4 + \nu)/(5n + 11)$ (regime D), respectively, where l, m, n, and ν are as defined above. An important empirical fact is that the charge filling ν inside channels lies approximately in the range $0.5 \lesssim \nu \lesssim 0.7$.

In some cases of f, the value of l, m, or n can be almost uniquely identified by combining this restriction on ν and the above relations. However, in general, there can be more than one value of l, m, or n compatible with the above range of ν and the relations. In those ambiguous cases, we performed simulations on the lattices with sizes commensurable with each of the candidate striped states. By this procedure, the system with lattice size that is not commensurate with the true ground state configuration usually results in defective configurations lacking in global order, thereby allowing us to identify the stable configuration. We could identify by this method channel-striped configurations up to $l = 3$, $m = 3$, and $n = 4$. As the value of f approaches near $1/3$ (for example, $f \lesssim 0.34$) or f gets close to $2/5$ from below (for example, $0.395 \lesssim f < 0.4$), the unit cell of the channel-striped configuration gets larger, and we found it very hard to equilibrate the systems into some ordered configurations within reasonable computation time. In these limits, it is possible that there may exist many metastable states competing with striped configurations. Except for these extremes, for all the striped configurations we could identify, we confirmed the stability of the configurations.

We find that there exists in general another transition at lower temperature T_p corresponding to charge freezing inside partially filled channels. In order to check this, we calculated the inverse dielectric constant along two perpendicular diagonals to identify the transition temperatures. The wave vector dependent inverse dielectric constant is defined as [16], $\epsilon^{-1}(\vec{k}) = (1 - \frac{2\pi}{T\Omega k^2}\langle\rho_k\rho_{-k}\rangle)$, where $\rho_k \equiv \sum_{r_i} Q(\vec{r}_i)\exp(-i\vec{k}\cdot\vec{r}_i)$ is the Fourier component at wave vector $\vec{k}$ of the charge density, and $\Omega \equiv L^2$ is the total area of the system. By letting $\vec{k} \to 0$ for a given direction of the wave vector, one can obtain the long wavelength limit of the inverse dielectric constant along a specific direction.

Figure 3 shows the dependence of the inverse dielectric constant along parallel and perpendicular to the stripes, respectively, for $f = 13/35$. We can clearly see that there exists, in addition to the transition at $T_c \simeq 0.32$ corresponding to the onset of striped order, an intermediate regime of temperature where the dielectric constant exhibits asymmetry due to the channel-striped structures. Also, the system is seen to undergo another transition at lower temperature $T_p \simeq 0.015$ (determined as the temperature where the inverse dielectric constant changes most rapidly). Figure 4 shows the dependence of the inverse dielectric constant along parallel to the stripes for various values of f in regime B, where a wide variation is seen in the temperature dependence of the inverse dielectric constant.

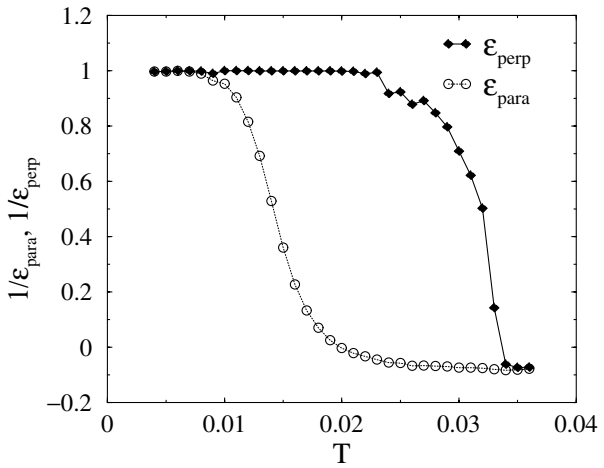

FIG. 3. Inverse dielectric constants along parallel (diamonds) and perpendicular (circles) to the stripes for $f = 13/35$ and $L = 35$ versus temperature. We can clearly see an anisotropy of the inverse dielectric constants.

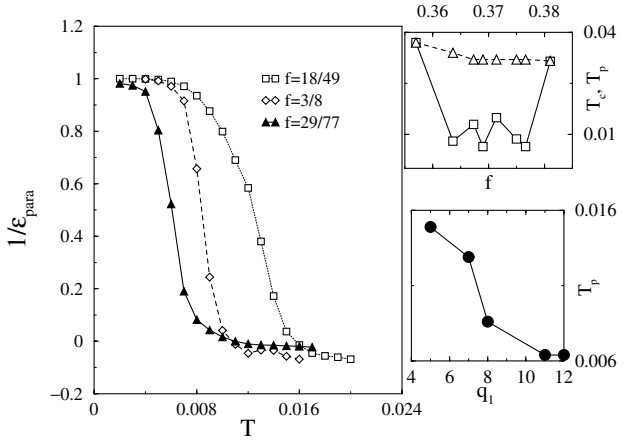

FIG. 4. Inverse dielectric constants along parallel to the stripes for $f = 18/49$ ($\nu = 4/7$), $f = 3/8$ ($\nu = 5/8$), and $f = 29/77$ ($\nu = 7/11$), respectively. These are chosen from regime B. Top right: Transition temperatures T_c (triangles) and T_p (squares) versus the charge filling ratio f. Bottom right: The dependence of T_p on the denominator q_1 of $\nu = p_1/q_1$.

Shown in top right of Fig. 4 is the dependence of the two transition temperatures on $f = p/q$ in regime B where the higher transition T_c is seen to depend on the values of f smoothly, while the lower transition temperature T_p exhibits sensitive dependence on f. From the bottom right of Fig. 4 which is a plot of T_p versus the integer denominator q_1 of the charge number density $\nu \equiv p_1/q_1$ within channels, one can recognize that T_p decreases monotonically as q_1 increases. This is another commensuration effect coming from the rationality of the particle number density within channels each of which forms effectively a one-dimensional lattice gas system. The freezing transition T_p corresponds basically to the freezing of charges within individual channels into the pattern given in Refs. [1,2] (at least for the values of f considered in this work). For some cases of f (e.g., $f = 13/35$), this freezing is found to be accompanied by a unique long range correlation between charges inside different channels. In general, however, the relative arrangement of charges within different channels could depend on the history of annealing, presumably due to some degeneracies or near degeneracies in the energy of the configurations.

Now we are left with the region of $f_{c3} < f < 1/2$. Even though we have not investigated the ordered configurations extensively for all values of f in this regime, we could see, from our simulations for some typical rational values of f in this regime, that the low-temperature configuration no longer shows striped patterns but rather consists of regular arrays of hole defects upon $f = 1/2$ checkerboard configurations [9,17].

In summary, we have shown numerically that the 2D LCG on a square lattice exhibits a simple regularity in its striped charge configuration at low-temperatures for f in a large part of the range $1/3 < f < 1/2$ which consists of simple combinations of four basic striped patterns characterized by the existence of partially filled diagonals. In general, there exists another transition at a lower temperature T_p corresponding to the freezing within partially filled channels. It would be interesting to observe these striped charge patterns experimentally, e.g., in arrays of ultrasmall tunnel junctions or in the macroscopic systems of dielectric charged spheres [18] under periodic pinning potentials.

This work was supported by the Korea Research Foundation Grants No. KRF-1999-015-DP0098 (S. J. L. and B. K.) and No. KRF-1998-15-D00089 (J. R. L.). B. K. was also supported by Korea Research Foundation Grant No. KRF-2000-008-2.

[1] J. Hubbard, Phys. Rev. B **17**, 494 (1978).
[2] V. L. Pokrovsky and G. V. Uimin, J. Phys. C **11**, 3535 (1978).
[3] P. Bak and R. Bruinsma, Phys. Rev. Lett. **49**, 249 (1982).
[4] See articles in *Phase Transitions in Surface Films,* edited by J. G. Dash and J. Ruvalds (Plenum, New York, 1980).
[5] See articles in *Coherence in Superconducting Networks,* edited by J. E. Mooij and G. Schön [Physica (Amsterdam) **152B**, 1–299 (1988)].
[6] For lattice Coulomb gas, see P. Minnhagen, Rev. Mod. Phys. **59**, 1001 (1987); L. P. Kadanoff, *Statistical Physics* (World Scientific, Singapore, 2000), Chaps. 15–17.
[7] J. Villain, J. Phys. (Paris) **36**, 581 (1975); J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B **16**, 1217 (1977).
[8] S. Teitel and C. Jayaprakash, Phys. Rev. Lett. **51**, 1999 (1983); R. Theron, J. B. Simond, J. L. Gavilano, Ch. Leemann, and P. Martinoli, Physica (Amsterdam) **165B&166B**, 1641 (1990); R. Theron *et al.,* Phys. Rev. Lett. **72**, 562 (1994).
[9] M. Franz and S. Teitel, Phys. Rev. B **51**, 6551 (1995); S. Teitel, in *Proceedings of the Sitges Conference on Glassy Systems,* edited by M. Rubi and C. Perez-Vincente (Springer-Verlag, Berlin, 1997); J. P. Straley and G. M. Barnett, Phys. Rev. B **48**, 3309 (1993).
[10] T. C. Halsey, Phys. Rev. B **31**, 5728 (1985).
[11] C. Denniston and C. Tang, Phys. Rev. B **60**, 3163 (1999).
[12] M. R. Kolahchi, Phys. Rev. B **59**, 9569 (1999); M. R. Kolahchi and H. Fazli, Phys. Rev. B **62**, 9089 (2000).
[13] P. Gupta, S. Teitel, and M. J. P. Gingras, Phys. Rev. Lett. **80**, 105 (1998).
[14] For details, see J.-R. Lee and S. Teitel, Phys. Rev. B **46**, 3247 (1992).
[15] For finite screening length λ, we find that there exists a threshold magnitude $\lambda = \lambda_c$ ($\lambda_c \simeq 1.6$ for $f = 13/35$) above which the channel-striped configuration remains stable, but it becomes unstable below λ_c.
[16] G. S. Grest, Phys. Rev. B **39**, 9267 (1989); P. Minnhagen and G. G. Warren, Phys. Rev. B **24**, 2526 (1981).
[17] S. J. Lee, B. Kim, and J.-R. Lee, Phys. Rev. E **64**, 066103 (2001).
[18] Y. Choi, K. Kim, and H. K. Pak, Physica (Amsterdam) **281A**, 99 (2000).