Patterns of Striped Order in the Classical Lattice Coulomb Gas

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We obtain via Monte Carlo simulations the low temperature charge configurations in the lattice Coulomb gas on square lattices 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.

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Competition between periodic pinning potential and repulsive inter-particle interactions often generate interesting frustration effects on the equilibrium properties of particle systems resulting in diverse commensurate or incommensurate phases [1,2]. In the simplest case of one dimensional system on a lattice, there exists a well known prescription of obtaining the ground state configuration $\mathbb{L}$ for a given particle density provided that the inter-particle potential is convex and vanishing at infinity. In two dimensions, systematic or analytic results are scarce [3].

One of the extensively studied model systems in two dimensions is the classical lattice Coulomb gas (LCG), where a fraction $f = p/q$ ($p$ and $q$ are relative primes) of the lattice sites are occupied by unit charges upon uniform neutralizing background $\mathbb{F}$. LCG appears in the vortex representation of the two dimensional Josephson junction arrays under uniform external magnetic field via Villain approximation [4] of the uniformly frustrated XY (UFXY) model, where the parameter $f$ corresponds to the ratio of the magnetic flux per unit plaquette and the superconducting flux quantum $\Phi_0 = hc/2e$. In these systems, physical properties such as transition temperatures or critical currents can depend sensitively on (the rationality of) the value of the frustration parameter $f$ due to the commensuration effect [4].

In spite of many years of research effort, there still remains wide range of $f$ parameter (notably for $1/3 < f < 1/2$) for which not much is known in terms of equilibrium properties. Even the ground state configurations are known only for some limited cases of values of $f$, especially for low order rationals [5,6]. In this paper, we report simulation results on the low temperature ordered structures of LCG on square lattices for $1/3 < f < 1/2$.

In the case of UFXY model on square lattices, Halsey proposed staircase states [6] as the low temperature ordered configurations with periodicity $q \times q$. However, the staircase state turns out to be the true ground state configuration only for some limited values of $f$ such as $f = 1/2, 1/3, 2/5, 3/8$, etc. More recent works on UFXY model [5] and LCG [7] shows that for $f = p/q$ near $1 - g$ ($g = (\sqrt{5} - 1)/2$) with $q$ large, the low temperature vortex configuration in the UFXY model can be different from the ordered charge configurations in LCG. Especially in the case of LCG on square lattices, it was shown [12] that there appear diagonal striped configurations with partially filled diagonals. However, the exact patterns of low temperature charge configurations for general $f$ of dense charge filling have not been enumerated yet.

In this paper, we find numerically for LCG on square lattices with $f$ in a large part of the range $1/3 < f < 1/2$, that, below a first order transition temperature $T_c$, the charge 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. $T_c$ is found to be only weakly dependent on $f$. Below $T_c$, there exist in general a temperature range where the charges within partially filled diagonal channels are disordered (thus mobile along channels). We found that there exist another transition at a lower temperature $T_p$ at which freezing of charges within partially filled channels occur. An interesting result is that 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 [1] is described by the following Hamiltonian,

$$H_{CG} = \frac{1}{2} \sum_{ij} Q_i G(r_{ij}) Q_j$$

(1)

where $r_{ij}$ is the distance between the sites $i$ and $j$, and the magnitude of charge $Q_i$ at site $i$ can take either $1$ 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’s function \( G(\vec{r}_{ij}) \) solves the equation \((\Delta^2 - \lambda^{-2})G(\vec{r}_{ij}) = -2\pi\delta_{\vec{r}_{ij},0}\), where \( \Delta^2 \) is the discrete lattice Laplacian and \( \lambda \) is the screening length. For the case of usual Villain transformation of UFXY model, we obtain for the case of usual Villain transformation of UFXY model, we

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

where \( k \) 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 \( G(\vec{r}) \approx \ln r + i \). In this work, the presented results are all obtained for the case of \( \lambda \to \infty \).

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 moving it over to one of the nearest neighbor (NN) or next nearest neighbor (NNN) sites. An important aspect of our simulations is that one has to choose the lattice size appropriately in order to match the periodicity of the low temperature configuration (see below). If, otherwise, one chooses a lattice size that is incommensurate with the periodicity of striped patterns, then one ends up with defective charge configurations.

To begin with, let us present the four basic component patterns (Fig. 1) before going into the full description of the striped configurations. 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 single isolated diagonal filled with charges, that is neighbored by empty diagonals on both sides. Repetition of this pattern produces the ground state configuration for \( f = 1/3 \) with spatial periodicity three.

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 is essentially a partially filled diagonal enveloped by one filled diagonal on both sides at second neighbor diagonal position, which may be termed as a channel structure. This can form a basis of a periodic configuration with spatial lattice periodicity seven. Lastly, the fourth component pattern (IV) can be denoted by \( 01010p010 \). This is component pattern consisting of a partially filled diagonal bounded by two type II stripe patterns on both sides. This can form a basis of a periodic configuration with spatial lattice periodicity eleven.

We are now in a position to be able to give a detailed description of the low temperature charge patterns. We may identify four regimes for the striped charge configuration. We may call these by regime \( A, B, C, \) and \( D \) respectively. Fig. 2 shows typical representative configuration in each of the four regimes.

In regime \( A \) that is bounded by \( 1/3 \lesssim f \lesssim f_{c1} \) \( (f_{c1} \approx 0.357) \), 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 (I\ III) forms a basic unit, repetition of which forms the whole charge configuration. We can easily see that the lattice periodicity of the ordered stripe configuration is equal to \( p_A = 3l + 7 \).

As \( l \) approaches infinity, we recover the case of \( f = 1/3 \). As the value of \( f \) increases within regime \( A \), the value of \( l \) decreases monotonically in step-like manner. Therefore, regime \( A \) is further divided into sub-regimes each of which is characterized by a positive integer \( l \).

Regime \( B \) covers the region \( f_{c1} \lesssim f \lesssim f_{c2} \) \( (f_{c2} \approx 0.381) \), 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 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 (II\ III) forms 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 step-like manner. The case of \( f = 2/5 \) corresponds to the limit of \( m \to \infty \).

Regime \( D \) corresponds to \( 2/5 < f \ll f_{c3} \) \( (f_{c3} \approx 0.425) \), 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 II\ IV. We see that the lattice periodicity of the ordered stripe configuration in regime \( IV \) is equal to \( p_D = 5n + 11 \). As the value of \( f \) increases within regime \( D \), the value of \( n \) decreases monotonically in step-like manner.

Note that the periodicity in the above refers to the periodicity of the filled diagonals only, neglecting the true periodicity including the charge configurations within the partially filled diagonals. The true spatial periodicity of the charge configurations can be many times larger than the stripe periodicity since we also have to take into account the correlation of charge configurations between different partially filled channels.

For any given value of \( f \), we can easily obtain the
filling density $\nu$ inside the partially filled channel using the relations $f = (l + 2 + \nu)/(3l + 7)$ (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 $\nu$ are as defined above. As the value of $f$ continuously increases within one sub-regime, the system in the low temperature stable configuration simply adjusts itself by accommodating the extra number of charges into the partially filled diagonal channels and thereby changing the charge filling $\nu$ within the channels.

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 that, 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 follows [14],

$$\varepsilon^{-1}(\vec{k}) = \left( 1 - \frac{2\pi}{T\Omega k^2} < \rho_k \rho_{-k} > \right),$$

(3)

where $\rho_k \equiv \sum_{r_i} Q(r_i) \exp(-i\vec{k} \cdot \vec{r}_i)$ 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 $k \to 0$ 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 $T_c \approx 0.32$ corresponding to the onset of striped order, 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 $T_p \approx 0.014$ (determined rather arbitrarily as the temperature where the inverse dielectric constant is equal to 0.4). 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 parallel to the channels.

Shown in Fig. 5 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 inset of Fig. 5 where 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 if we neglect the interaction between different channels. The arrangement of charges within each channel was found to follow the pattern given in ref. [1] and [2] at least for the values of $f$ considered in this work.

One can ask what determines the boundary value of $f$ and $\nu$ for each of the sub-regimes, in other words, what is the stability criterion for each pattern of the striped configuration. Even though an analytic formula cannot be given, our simulations suggest that the criterion of determining the crossover point between two neighboring subregimes is related to the electrostatic stability which is determined by the filling density inside the partially filled channel. We found numerically that for any given value of $f$ the filling density $\nu$ in the channel approximately satisfies the inequality $0.4 \lesssim \nu \lesssim 0.7$. For a given sub-regime, possible values of $\nu$ were always within this bound. Beyond some threshold value $\nu_c$ of $\nu$ that is within the above bound, electrostatic instability begins to set in, and rearrangement of the whole charge configuration occurs in order to form a new stable ordered patterns.

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 some of our annealing simulations for 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. If we suppose that $f = 1/2 - \alpha \equiv (1 - p_2/q_2)/2$ with $p_2$ and $q_2$ relative primes, then we can easily see that $f' = p_2/q_2 \equiv 2\alpha$ represents the density of hole defects upon the $f = 1/2$ checkerboard configuration. Therefore, we can suspect that the low temperature defect configuration in this regime will be equivalent to the charge configuration of lattice Coulomb gas with $f = f'$. We could confirm this expectation for a few cases of $f$ [13,14].

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 filling factor $f$ in a large part of the range $1/3 < f < 1/2$ which is characterized by the existence of partially filled diagonals. The low temperature ordered configuration consists of a simple combinations of four basic striped patterns. 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 regular square arrays of ultrasmall tunnel junctions. It may also be possible to observe similar patterns in the macroscopic systems of dielectric charged spheres [10] under periodic pinning potentials.

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FIGURE CAPTIONS

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 $\nu$ of the sites are filled with positive charges.

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.

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

Fig. 4. Inverse dielectric constant along parallel to the stripes for various values of charge number density $\nu$ within channels. All of the systems shown are chosen from regime B.

Fig. 5. Transition temperatures (both $T_c$ and $T_p$) versus the charge filling ratio $f$. Inset shows the dependence of $T_p$ on the denominator $q_1$ of $\nu = p_1/q_1$.
Lee, et al
Lee, et al
Lee, et al.
